

# *Appendix*

## BUFFERS, REAGENTS, SOLUTIONS

| Sl No. | Buffer   | Concentration |
|--------|--|---------------|
| I.     | <b>Phosphate buffer saline (pH 7.4)</b>          |               |
|        | NaCl   | 8 gm/L        |
|        | KCl  | 0.2 gm/L      |
|        | Na <sub>2</sub> HPO <sub>4</sub>                 | 1.42 gm/L     |
|        | KH <sub>2</sub> PO <sub>4</sub>                  | 0.24 gm/L     |
| II.    | <b>Sodium phosphate buffer 1M (pH 8.0)</b>       |               |
|        | 1 M Solution of Na <sub>2</sub> HPO <sub>4</sub> | 53 ml/L       |
|        | 1 M Solution of Na <sub>2</sub> PO <sub>4</sub>  | 947 ml/L      |
| III.   | <b>Sodium phosphate buffer 1M (pH 6.5)</b>       |               |
|        | 1 M Solution of Na <sub>2</sub> HPO <sub>4</sub> | 685 ml/L      |
|        | 1 M Solution of Na <sub>2</sub> PO <sub>4</sub>  | 315 ml/L      |
| IV.    | <b>Sodium phosphate buffer 1M (pH 7.0)</b>       |               |
|        | 1 M Solution of Na <sub>2</sub> HPO <sub>4</sub> | 390 ml/L      |
|        | 1 M Solution of Na <sub>2</sub> PO <sub>4</sub>  | 610 ml/L      |
| V.     | <b>Potassium phosphate buffer 1M (pH 7.5)</b>    |               |
|        | K <sub>2</sub> HPO <sub>4</sub>                  | 69.67 gm/L    |
|        | KH <sub>2</sub> PO <sub>5</sub>                  | 27.22 gm/L    |
| VI.    | <b>Tris KCL buffer</b>                           |               |
|        | KCL  | 74.55 gm/L    |
|        | Tris   | 121.14 gm/L   |
| VII.   | <b>Normal Saline</b>                             |               |
|        | NaCl   | 0.9 mg/L      |
| VIII.  | <b>Lysis buffer</b>                              |               |
|        | Tris-Cl (pH 8.0)                                 | 50mM          |
|        | NaCl   | 150mM         |
|        | Nonidet P-40                                     | 1X            |
|        | Sodium deoxycholate                              | 0.50%         |
|        | SDS  | 0.10%         |
|        | Sodium orthovanadate                             | 1mM           |
|        | NaF  | 1mM           |
|        | Protease inhibitor                               | 1X            |

|       |  |           |
|-------|--|-----------|
| IX.   | <b>Loading buffer (2X)</b>                           |           |
|       | Tris-Cl (pH 6.8)                                     | 100 mM    |
|       | SDS  | 4%        |
|       | Bromophenol blue                                     | 0.20%     |
|       | Glycerol   | 20%       |
|       | Dithiothreitol                                       | 200 mM    |
| X.    | <b>Running buffers (1x) (pH 8.3)</b>                 |           |
|       | Tris base  | 3 gm/L    |
|       | Glycine  | 14.4 gm/L |
|       | SDS  | 1 gm/L    |
| XI.   | <b>Transfer buffer (1X)</b>                          |           |
|       | Tris-Cl  | 25 mM     |
|       | Glycine  | 190 mM    |
|       | Methanol   | 20%       |
| XII.  | <b>Wash buffer (1X)</b>                              |           |
|       | Tris-Cl (Ph 7.5)                                     | 20 Mm     |
|       | NaCl   | 150 Mm    |
|       | Tween 20   | 0.10%     |
| XIII. | <b>Blocking buffer</b>                               |           |
|       | Wash buffer  | 1X        |
|       | Non-fat milk powder                                  | 5%        |
| XIV.  | <b>Stripping buffer</b>                              |           |
|       | Glycine  | 15 gm/L   |
|       | SDS  | 1 gm/L    |
|       | Tween 20   | 1%        |
|       | $\beta$ - mercaptoethanol                            | 0.80%     |
| XV.   | <b>Griess reagent</b>                                |           |
|       | N-1-naphthylethylenediamine dihydrochloride in water | 50%       |
|       | Sulfanilamide in 5% phosphoric acid                  | 50%       |

# *Annexures*



भारत सरकार / GOVERNMENT OF INDIA  
पर्यावरण एवं वन मंत्रालय / MINISTRY OF ENVIRONMENT AND FORESTS  
संयुक्त निदेशक कार्यालय / OFFICE OF THE JOINT DIRECTOR  
भारतीय वनस्पति सर्वेक्षण / BOTANICAL SURVEY OF INDIA  
पूर्वी क्षेत्रीय केन्द्र / EASTERN REGIONAL CENTRE  
शिलांग-793 003 / SHILLONG-793003



दूरभाष /Telephone: 0364- 2223971, 2223618 ई-मेल / e-mail-bsibsishll@yahoo.co.in Telefax: 0364 -2224119

No.BSI/ERC/Tech./Plant Iden./2015/ 306 ,

Date : 03-08-2015

To

Anowar Hussain  
Research Scholar  
Department of Molecular Biology and Biotechnology  
Tezpur University,  
Napaam, Tezpur -786028, Assam

Subject : Identification and authentication of plant species.

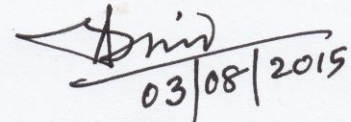
Dear Hussain,

With reference to your letter No. Nil dated 30-07-2015 regarding the subject cited above, I am to inform you that your plant specimens have been identified and confirmed as below:

1. *Phlogacanthus thyrsiflorus* Nees (Family-Acanthaceae) (TU/MBBT/AMR/PS/02),
2. *Nyctanthes arbor-tristis* L. (Family-Oleaceae) (TU/MBBT/AMR/PS/03)
3. *Alstonia scholaris* (L.) R.Br. (Family Apocynaceae) (TU/MBBT/AMR/PS/04)
4. *Basella alba* L. (Family Basellaceae) (TU/MBBT/AMR/PS/05)

Thanking you.

Yours Sincerely,

  
03/08/2015

(डॉ ए. ए. माओ) /Dr. A.A. Mao  
वैज्ञानिक ड / Scientist-'E' & Head of Office



DEPARTMENT OF BOTANY  
GAUHATI UNIVERSITY

Gopinath Bardoloi Nagar, Guwahati - 781 014

☎ : 0361 - 2570530

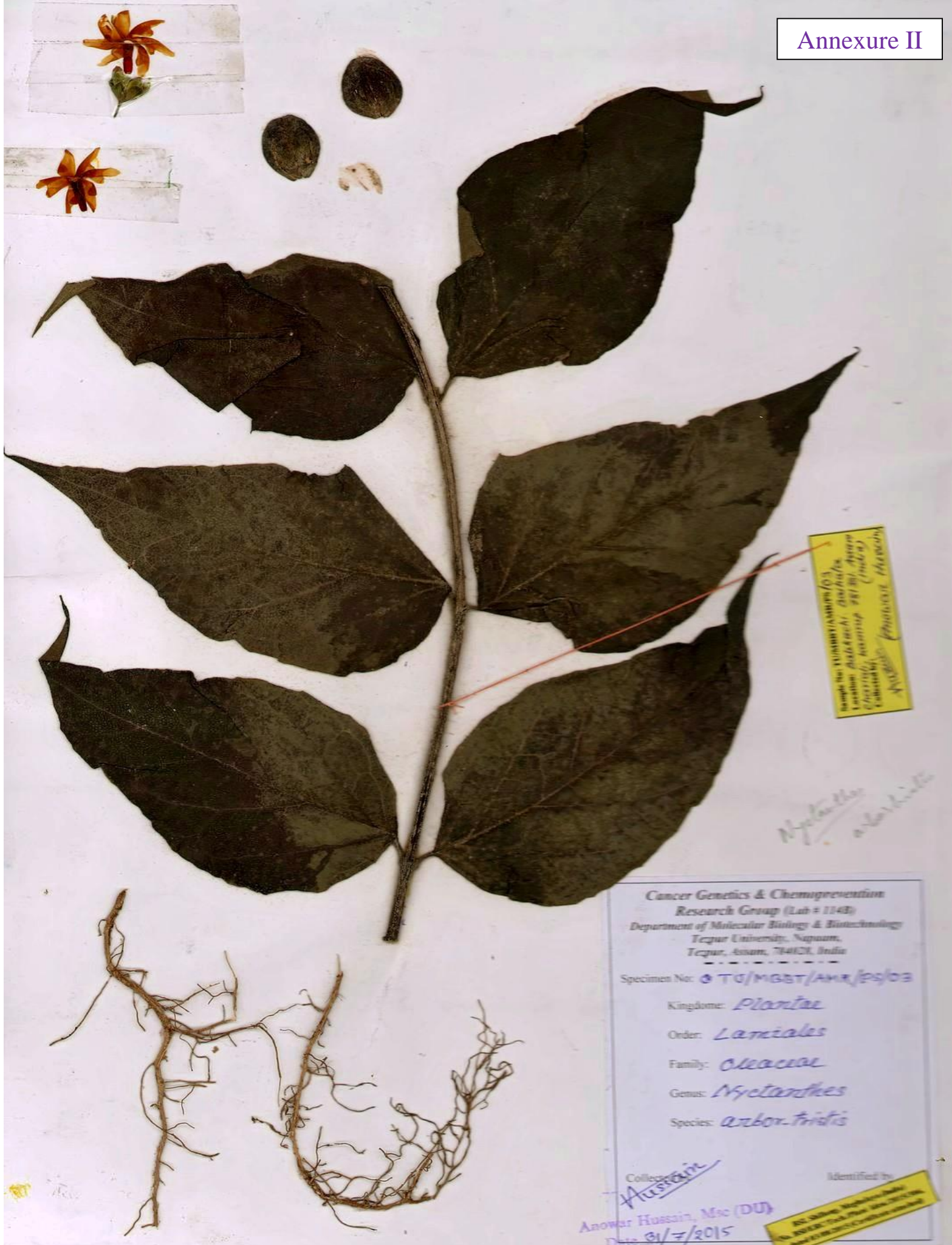
Ref. No. ....

Date : 16/5/11

This is to certify that the plants have been identified and authenticated by me.

Professor  
Department of Botany  
Gauhati University  
Guwahati-781014

- (i) Allium hookerii
- (ii) A. wallichii
- (iii) Adhatoda vesica
- (iv) Phlogacanthus sp.
- (v) Basella rubra
- (vi) Eryngium foetidum
- (vii) Melastoma scholarii
- (viii) Nyctanthus arborescens



Sample No: TUMSTIAMMIBS/03  
Name: Myctanthes arbor-tristis  
Location: Assam, India  
Collector: Anwar Hussain (DU)  
Date: 31/3/2015

*Myctanthes arbor-tristis*

Cancer Genetics & Chemoprevention  
Research Group (Lab # 114B)  
Department of Molecular Biology & Biotechnology  
Tezpur University, Nagaon,  
Tezpur, Assam, 784021, India

Specimen No: **03** TU/MBBT/AMR/PS/03


Kingdom: *Plantae*  
Order: *Lamiales*  
Family: *Celastraceae*  
Genus: *Myctanthes*  
Species: *arbor-tristis*

Collected by: *Anwar Hussain*  
Identified by: *Anwar Hussain, Msc (DU)*  
Date: *31/3/2015*

For Sliding, Scanning, etc.  
Dr. Anwar Hussain, Msc (DU)  
anwarhussain@tezpuruniv.ac.in



*Phlogacanthus tubiflorus*  
*H. yonishanus*

|   |            |
|---|------------|
|  <b>GUWAHATI UNIVERSITY : ASSAM</b> |            |
| Flora of _____  |            |
| Coll No. _____  | Date _____ |
| Family _____  |            |
| Genus & Species _____   |            |
| Locality _____  |            |
| Habitat _____   |            |
| Distribution _____  |            |
| Description _____   |            |
| Vern Name & Use _____   |            |
| Photo Date _____  |            |
| Collector _____   |            |





Sample No: TUMBBT/AMR/PS/02  
Location: Badkuchi, Barhala,  
Charrai, Kamrup, 781051, Assam  
(India)  
Collected by:  
A. S. Das (Ph.D. student, Assam)

*Phlogacanthus thysiflorus*

Cancer Genetics & Chemoprevention  
Research Group (Lab # 114B)  
Department of Molecular Biology & Biotechnology  
Tezpur University, Napaam,  
Tezpur, Assam, 784028, India

Specimen No: TU/MBBT/AMA/PS/02

Kingdom: *Plantae*

Order: *Lamiales*

Family: *Acanthaceae*

Genus: *Phlogacanthus*

Species: *thysiflorus*

Assam  
Date: 31/07/2015



## TEZPUR UNIVERSITY

Office of the Dean, Research & Development  
Napaam::Tezpur - 784 028::Assam::India

No. DoRD/TUEC/10-14/4361

Date: 28.03.2014

To  
✓ Dr. A. Ramteke  
Department of MBBT  
Tezpur University

Sub: Research proposal submitted to TUEC.

Dear Dr. Ramteke,

This is with reference to the research proposal entitled "Use of isolated lymphocytes as a test model" which was submitted to the Tezpur University Ethical Committee for ethical clearance. The proposal was reviewed in the Tezpur University Ethical Committee (TUEC) meeting held on 30/09/2013. This is to inform you that the proposal has been accorded ethical approval.

Thanking you,

Yours sincerely,

*Charu Lata Mahanta*  
(C.L. Mahanta) 28/3/2014  
Chairperson, TUEC

Copy to:

1. Professor S. Baruah, Dept. of MBBT, Member Secretary, TUEC.

*Charu Lata Mahanta*  
(C.L. Mahanta) 28/3/2014  
Chairperson, TUEC

CERTIFICATE

This is certify that the project title "Chemopreventive potential of hydroalcoholic extract of selected ----- in Swiss albino mice"

has been approved by the IAEC.

C. L. Mahanta


Name of Chairman/Member Secretary IAEC:

Name of CPCSEA nominee:

Signature with date

Charm lata Mahanta  
21/4/2013

Chairman/Member Secretary of IAEC:

  
13/05



CPCSEA nominee:

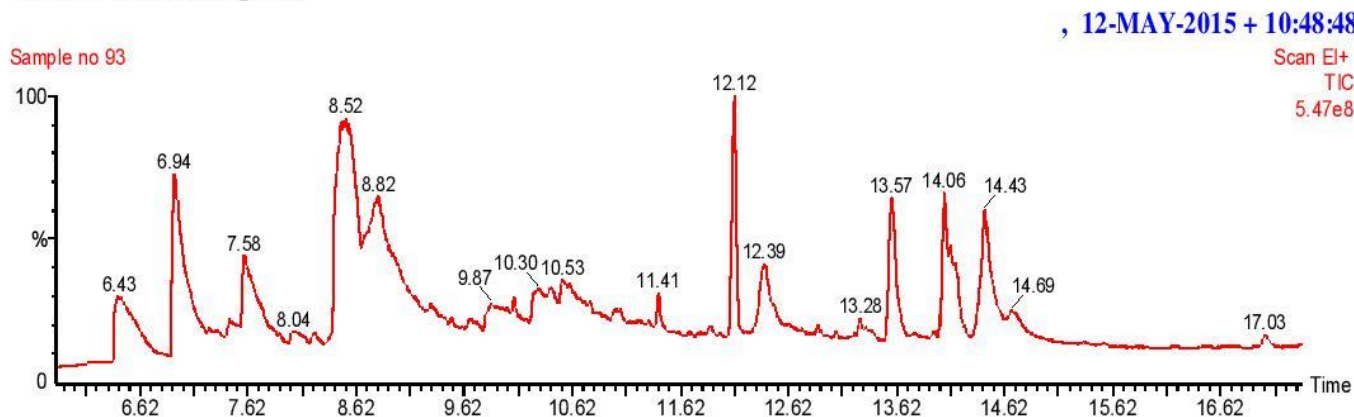
(Kindly make sure that minutes of the meeting duly signed by all the participants are maintained by Office)

**\*Components identified in FENA Sample (Code: 93)  
[GC MS study]:**

| No. | RT    | Name of the compound                         | Molecular Formulae                              | MW  | Peak Area % |
|-----|-------|--|---|-----|-------------|
| 1.  | 6.43  | 9-Oxa-bicyclo[3.3.1]nonane-1,4-diol          | C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>   | 158 | 8.59        |
| 2.  | 6.94  | 2,5-Methano-2H-furo[3,2-b]pyran, hexahydro-  | C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>   | 140 | 13.56       |
| 3.  | 7.58  | E-10-Pentadecenol                            | C <sub>15</sub> H <sub>30</sub> O               | 226 | 7.55        |
| 4.  | 8.52  | Dodecanoic acid, 3-hydroxy-                  | C <sub>12</sub> H <sub>24</sub> O <sub>3</sub>  | 216 | 26.41       |
| 5.  | 9.87  | Z-8-Methyl-9-tetradecenoic acid              | C <sub>15</sub> H <sub>28</sub> O <sub>2</sub>  | 240 | 2.14        |
| 6.  | 10.53 | α-D-Glucopyranose, 4-O-α-D-galactopyranosyl- | C <sub>12</sub> H <sub>22</sub> O <sub>11</sub> | 342 | 4.81        |
| 7.  | 11.41 | Cyclopentaneundecanoic acid, methyl ester    | C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>  | 268 | 0.78        |
| 8.  | 12.12 | Hexadecanoic acid, ethyl ester               | C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>  | 284 | 6.45        |
| 9.  | 12.39 | n-Hexadecanoic acid                          | C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>  | 256 | 5.44        |
| 10. | 13.28 | 9,12-Octadecadienoic acid (Z,Z)-             | C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>  | 280 | 0.47        |
| 11. | 13.57 | Phytol                                       | C <sub>20</sub> H <sub>40</sub> O               | 296 | 5.93        |
| 12. | 14.06 | 9,12-Octadecadienoic acid, ethyl ester       | C <sub>20</sub> H <sub>36</sub> O <sub>2</sub>  | 308 | 8.54        |
| 13. | 14.43 | Oleic Acid                                   | C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>  | 282 | 8.68        |
| 14. | 17.03 | E-11-Hexadecenoic acid, ethyl ester          | C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>  | 282 | 0.65        |

\*Parameters tested are not covered under the scope of NABL accreditation

### GCMS Chromatogram



Data Path : E:\GCMSD\2016\January\280116\  
 Data File : MSD.D  
 Acq On : 28 Jan 2016 12:44  
 Operator :  
 Sample : LEPT (B2604)  
 Misc :  
 ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e  
 Integrator: ChemStation

Method : E:\GC METHODA\HSRSSIM.M  
 Title : Pest-1

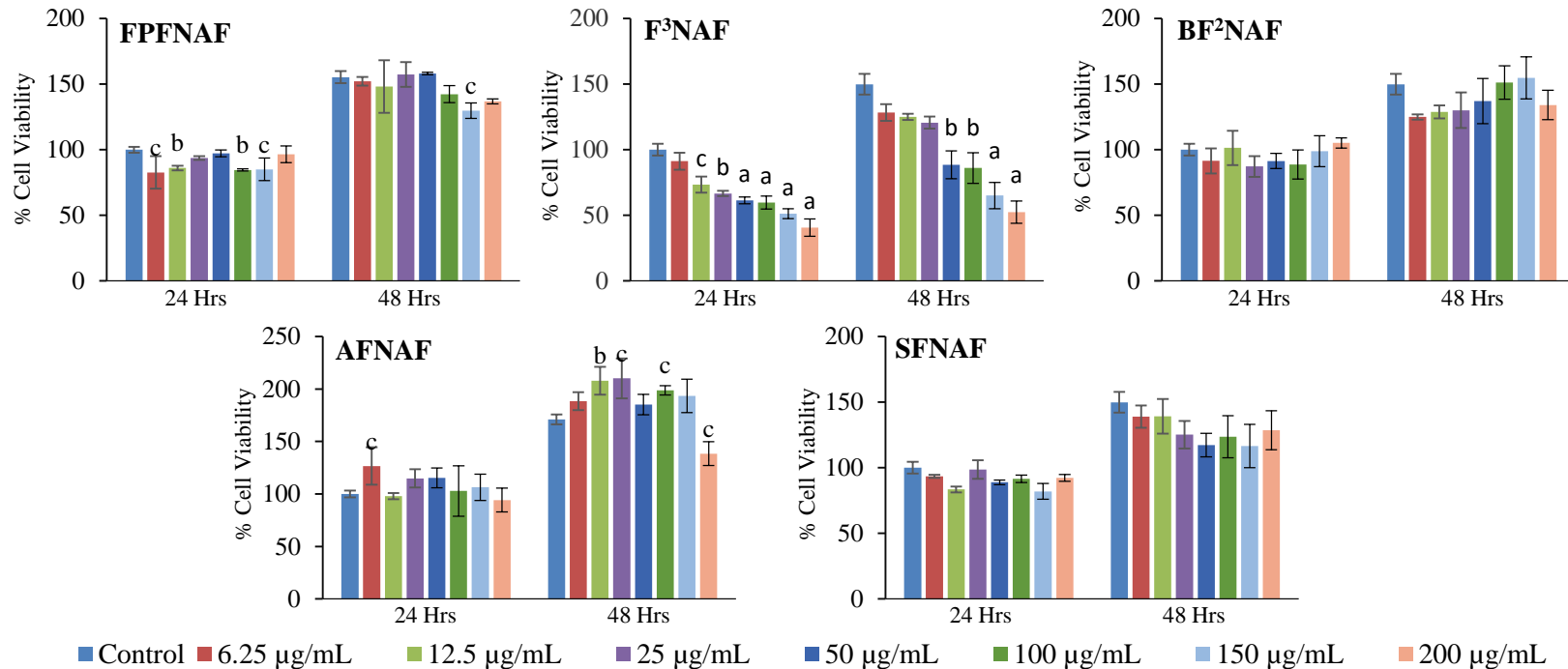
Signal : TIC: MSD.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 19.028   | 940        | 945      | 950       | M     | 38025       | 886421     | 0.24%        | 0.066%     |
| 2      | 22.505   | 1264       | 1275     | 1285      | M6    | 46259       | 2532159    | 0.69%        | 0.188%     |
| 3      | 24.121   | 1421       | 1429     | 1438      | M3    | 56069       | 3495912    | 0.96%        | 0.259%     |
| 4      | 25.502   | 1552       | 1560     | 1567      | M4    | 73247       | 3059185    | 0.84%        | 0.227%     |
| 5      | 26.581   | 1658       | 1663     | 1677      | PB 3  | 106477      | 3635055    | 1.00%        | 0.270%     |
| 6      | 31.721   | 2147       | 2151     | 2156      | M2    | 105750      | 2652348    | 0.73%        | 0.197%     |
| 7      | 34.795   | 2436       | 2443     | 2450      | PV    | 214111      | 5324459    | 1.46%        | 0.395%     |
| 8      | 35.298   | 2484       | 2491     | 2498      | M9    | 55857       | 1833026    | 0.50%        | 0.136%     |
| 9      | 35.668   | 2522       | 2526     | 2533      | M4    | 68406       | 1912264    | 0.52%        | 0.142%     |
| 10     | 36.466   | 2581       | 2602     | 2607      | BV    | 533363      | 23336284   | 6.40%        | 1.731%     |
| 11     | 37.442   | 2659       | 2695     | 2731      | PV 2  | 1655671     | 151879312  | 41.68%       | 11.269%    |
| 12     | 39.502   | 2884       | 2891     | 2898      | VV 4  | 156601      | 5724628    | 1.57%        | 0.425%     |
| 13     | 39.769   | 2908       | 2916     | 2921      | PV    | 2547477     | 87973225   | 24.15%       | 6.527%     |
| 14     | 39.904   | 2921       | 2929     | 2937      | VV 3  | 7945915     | 364352456  | 100.00%      | 27.034%    |
| 15     | 40.113   | 2944       | 2949     | 2964      | VV    | 1703522     | 49903275   | 13.70%       | 3.703%     |
| 16     | 40.423   | 2964       | 2978     | 2988      | PV    | 1674747     | 49380064   | 13.55%       | 3.664%     |
| 17     | 41.434   | 3068       | 3074     | 3082      | BV    | 136491      | 4220117    | 1.16%        | 0.313%     |
| 18     | 41.763   | 3100       | 3105     | 3110      | BV    | 164227      | 4215412    | 1.16%        | 0.313%     |
| 19     | 42.610   | 3180       | 3186     | 3192      | PV    | 239717      | 6750063    | 1.85%        | 0.501%     |
| 20     | 43.492   | 3264       | 3270     | 3286      | PV 2  | 154039      | 5114480    | 1.40%        | 0.379%     |
| 21     | 44.479   | 3357       | 3364     | 3396      | VV    | 519372      | 28653525   | 7.86%        | 2.126%     |
| 22     | 45.545   | 3457       | 3465     | 3471      | VV 6  | 142163      | 4963785    | 1.36%        | 0.368%     |
| 23     | 45.672   | 3471       | 3477     | 3492      | VB    | 160292      | 6164138    | 1.69%        | 0.457%     |
| 24     | 46.582   | 3557       | 3564     | 3569      | VV 2  | 367311      | 11401663   | 3.13%        | 0.846%     |
| 25     | 46.779   | 3577       | 3582     | 3589      | VV 2  | 252999      | 8506411    | 2.33%        | 0.631%     |
| 26     | 47.177   | 3611       | 3620     | 3640      | VV    | 851269      | 26276519   | 7.21%        | 1.950%     |
| 27     | 48.333   | 3724       | 3730     | 3733      | M2    | 217286      | 6843536    | 1.88%        | 0.508%     |
| 28     | 50.866   | 3955       | 3971     | 3994      | VV    | 1371456     | 78547020   | 21.56%       | 5.828%     |
| 29     | 51.342   | 4011       | 4016     | 4024      | VV    | 351237      | 12423054   | 3.41%        | 0.922%     |
| 30     | 53.196   | 4186       | 4192     | 4195      | VV 3  | 400602      | 16013991   | 4.40%        | 1.188%     |
| 31     | 53.787   | 4240       | 4248     | 4263      | VV 3  | 2641695     | 110287053  | 30.27%       | 8.183%     |
| 32     | 54.006   | 4263       | 4269     | 4275      | VV 4  | 362294      | 15509165   | 4.26%        | 1.151%     |
| 33     | 54.361   | 4296       | 4303     | 4313      | VV 7  | 271819      | 16508012   | 4.53%        | 1.225%     |
| 34     | 54.582   | 4313       | 4324     | 4337      | VV 4  | 707712      | 36449758   | 10.00%       | 2.704%     |
| 35     | 54.805   | 4337       | 4345     | 4352      | VV 5  | 616407      | 29548051   | 8.11%        | 2.192%     |
| 36     | 55.155   | 4361       | 4378     | 4390      | VV 2  | 2199482     | 100440912  | 27.57%       | 7.452%     |
| 37     | 55.553   | 4409       | 4416     | 4427      | VV 10 | 162412      | 8204699    | 2.25%        | 0.609%     |
| 38     | 55.979   | 4446       | 4457     | 4465      | VV 7  | 127760      | 7744369    | 2.13%        | 0.575%     |
| 39     | 56.552   | 4499       | 4511     | 4530      | VV 8  | 222191      | 16247543   | 4.46%        | 1.206%     |
| 40     | 57.855   | 4618       | 4635     | 4648      | VB 8  | 165628      | 9519854    | 2.61%        | 0.706%     |
| 41     | 59.736   | 4805       | 4814     | 4838      | VV 8  | 162023      | 12171130   | 3.34%        | 0.903%     |
| 42     | 60.149   | 4838       | 4853     | 4863      | PV 8  | 140666      | 7163072    | 1.97%        | 0.531%     |

Sum of corrected areas: 1347767404

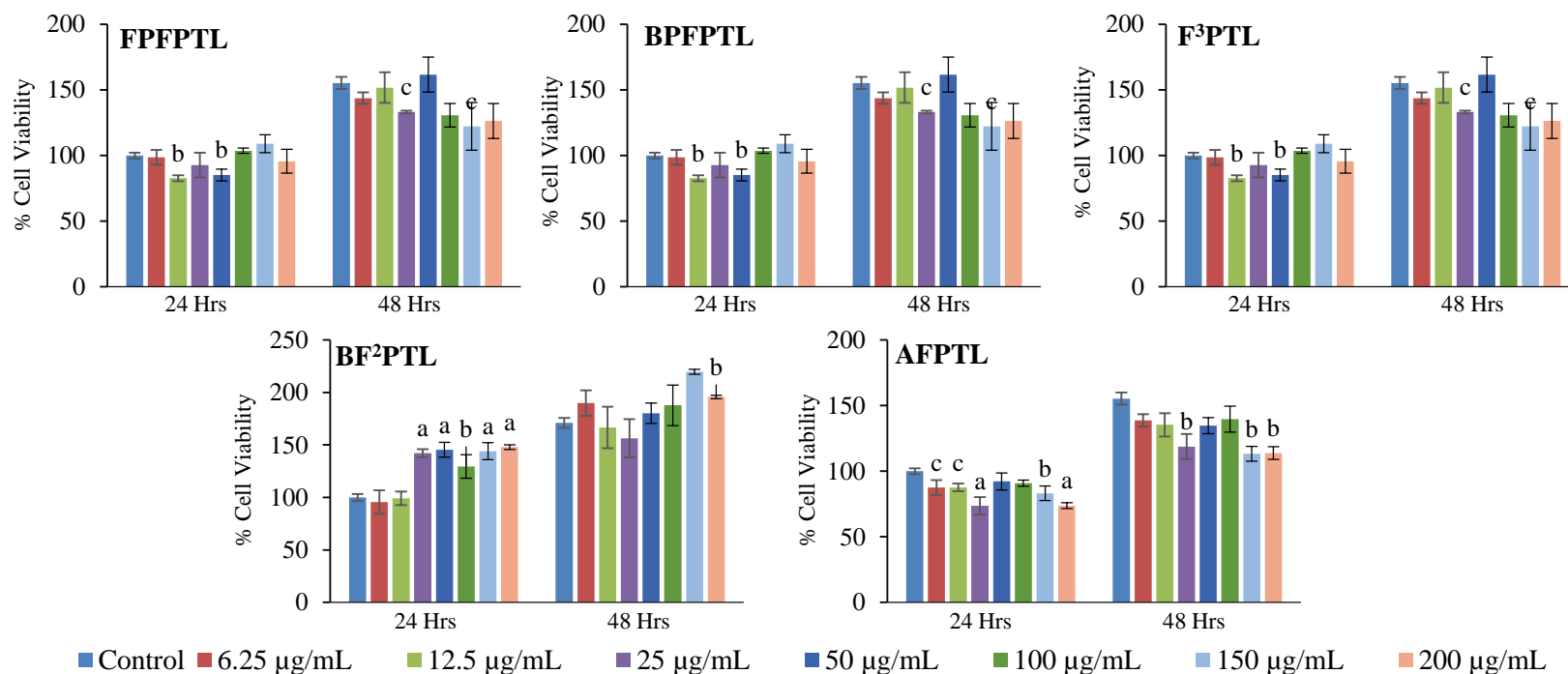
## Screening data

### Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human lung cancer H1299 cells



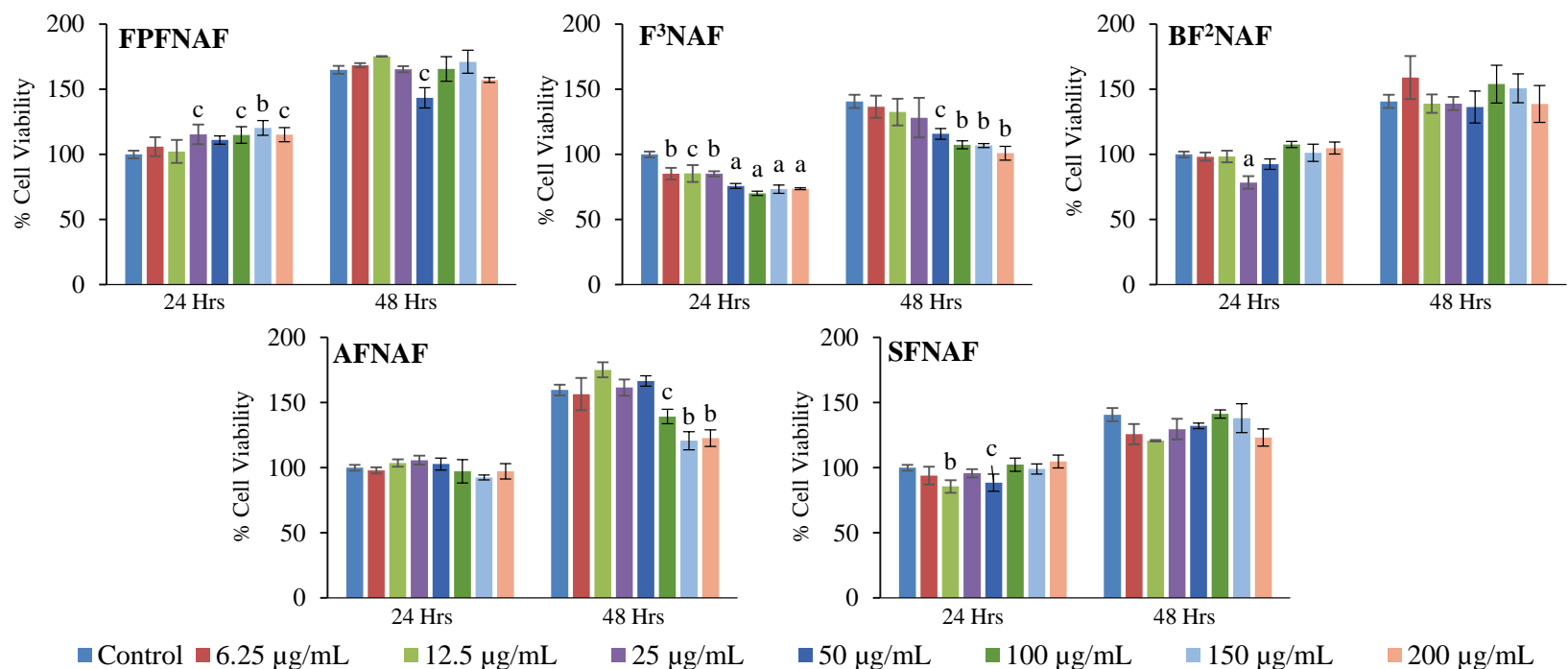
**Figure.** Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human lung cancer H1299 cells: H1299 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in 'Material and Methods', and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human lung cancer H1299 cells



**Figure.** Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human lung cancer H1299 cells: H1299 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in 'Material and Methods', and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

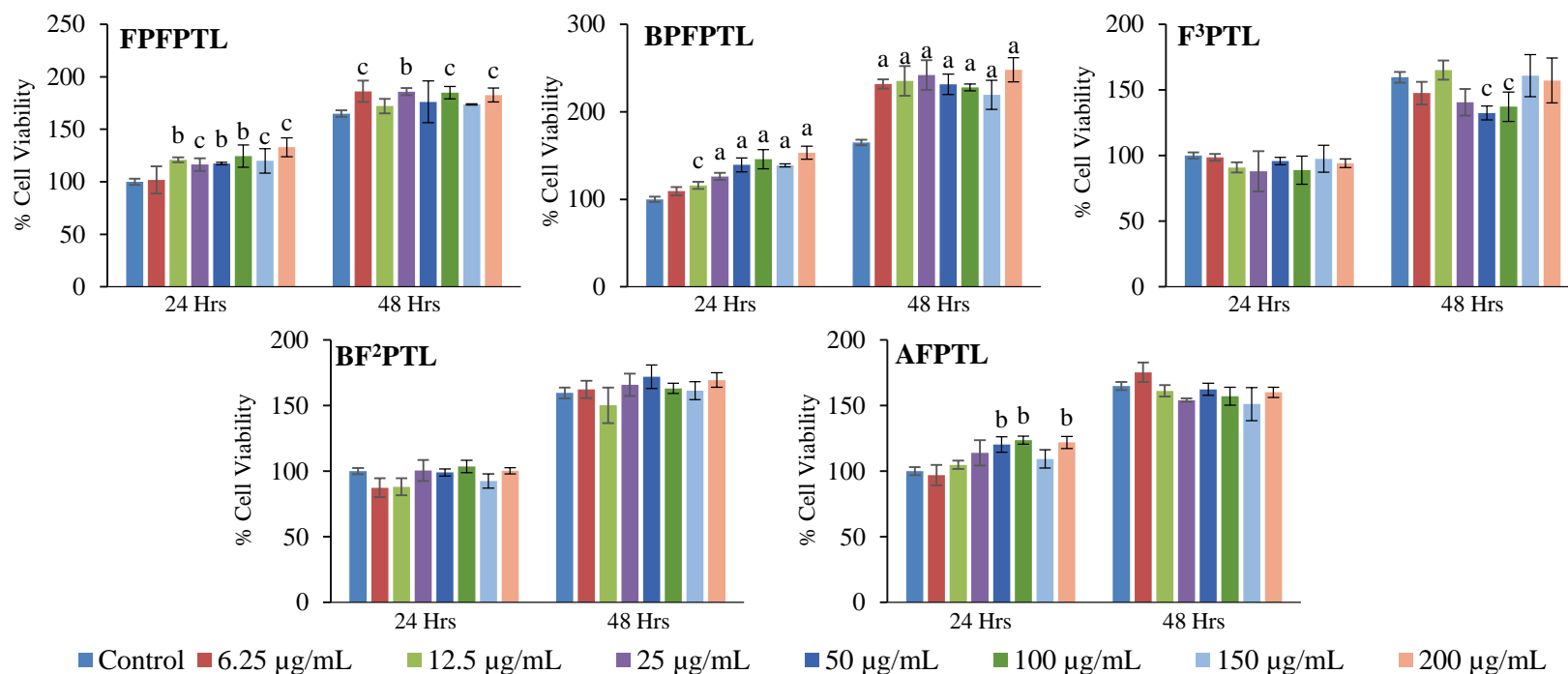
## Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human lung cancer A549 cells



**Figure.** Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human lung cancer A549 cells: A549 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in 'Material and Methods', and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

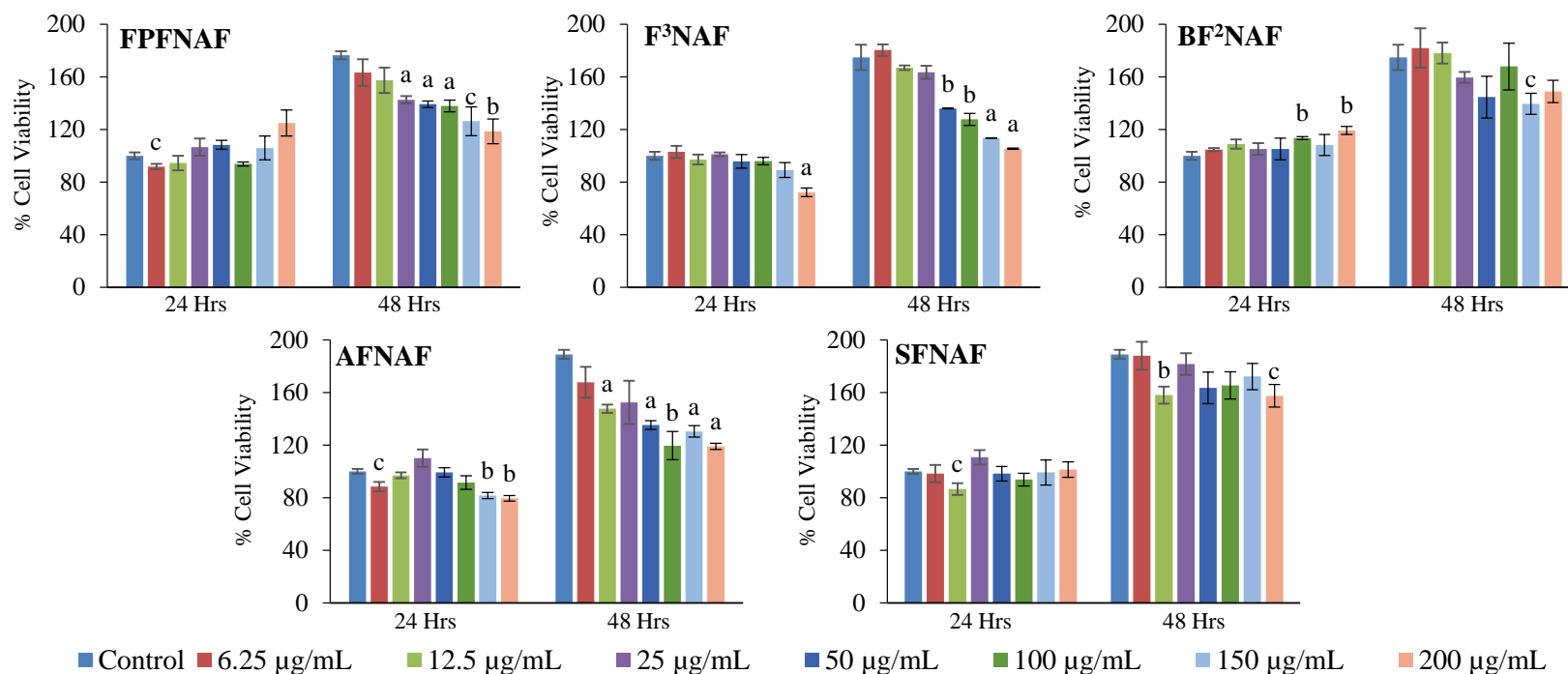


## Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human lung cancer A549 cells



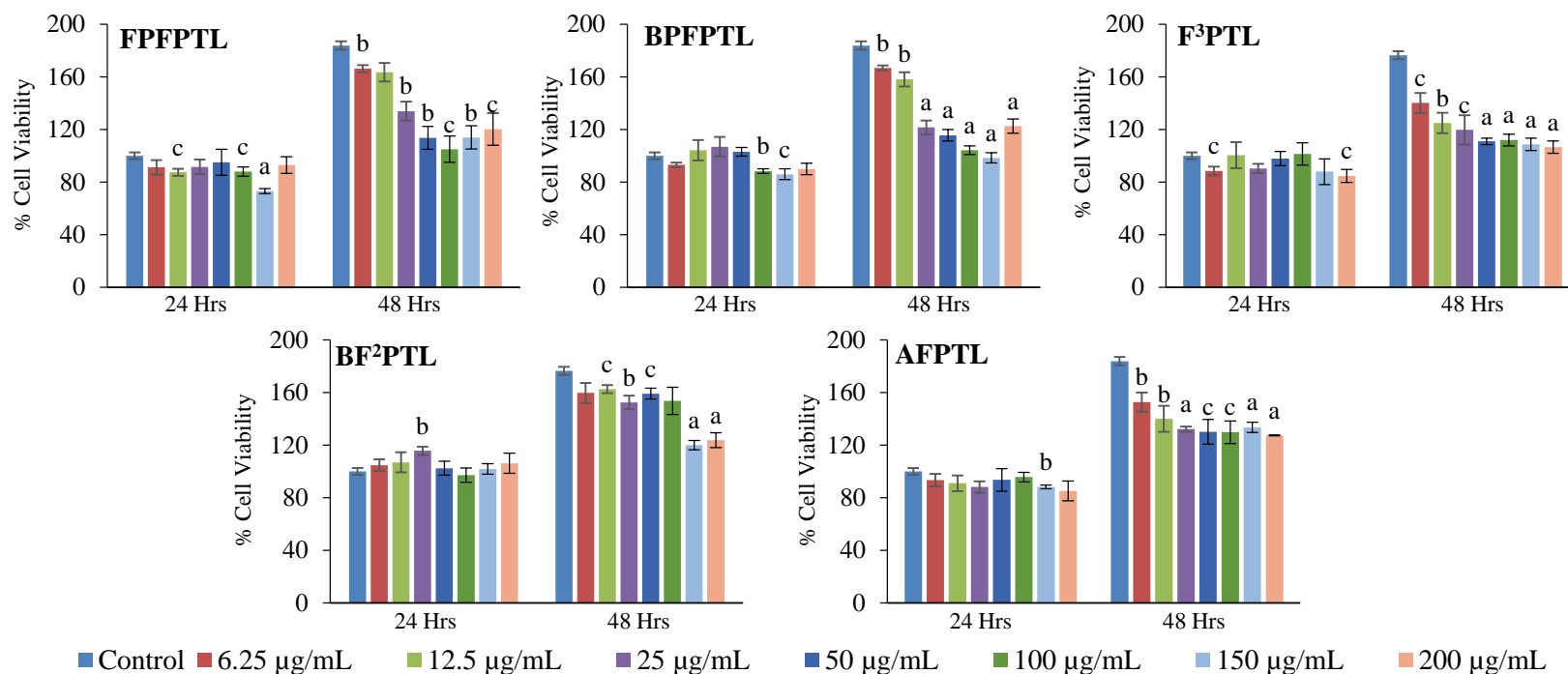
**Figure.** Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human lung cancer A549 cells: A549 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in ‘Material and Methods’, and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human prostate cancer PC3 cells



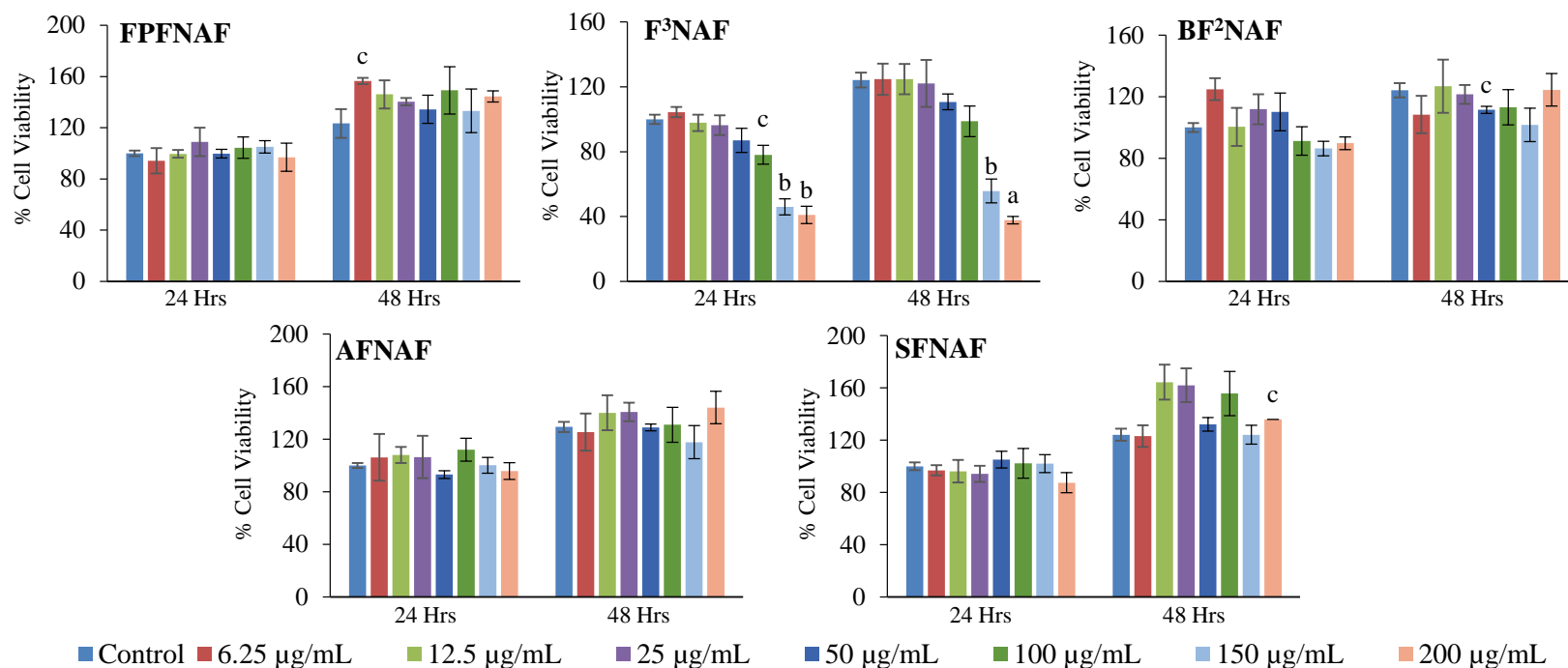
**Figure.** Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human prostate cancer PC3 cells: PC3 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in 'Material and Methods', and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Phlogacanthus thyriflorus* on the viability of human prostate cancer PC3 cells



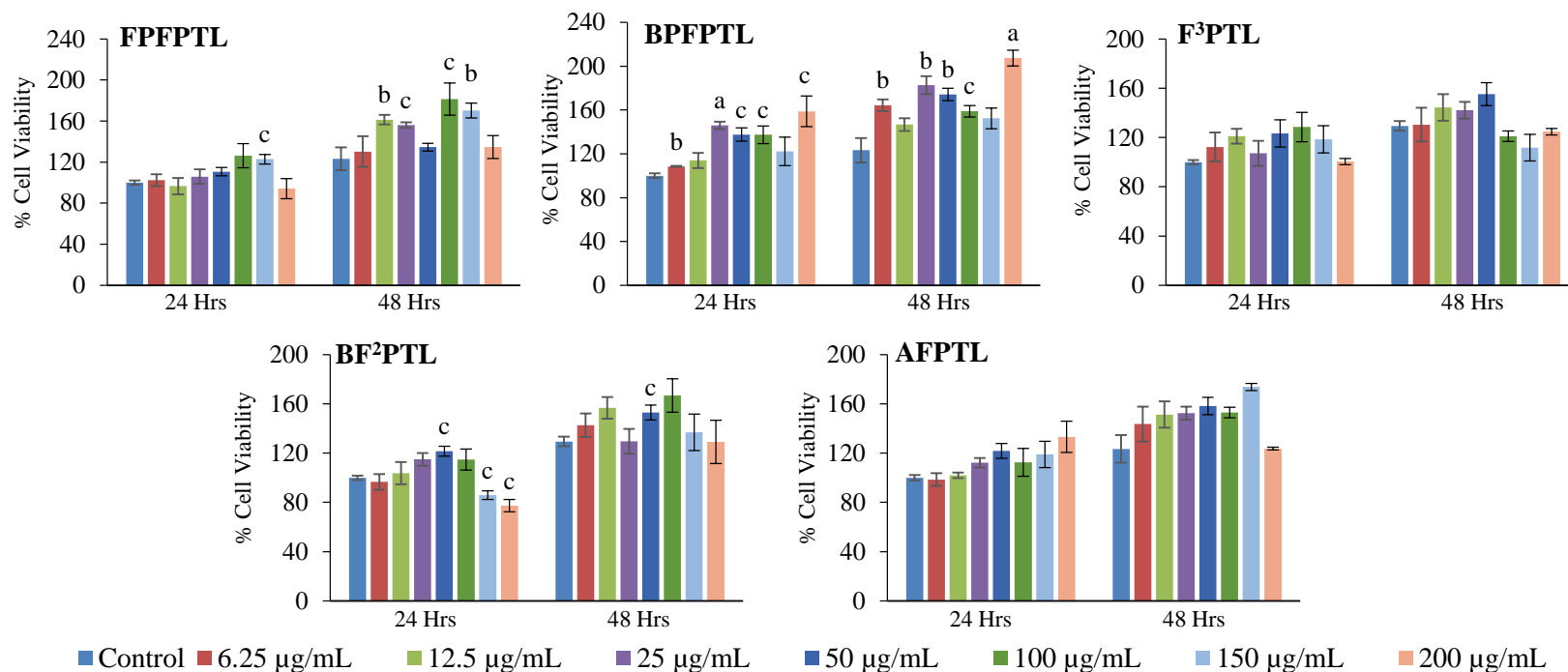
**Figure.** Effects of different fractions of *Phlogacanthus thyriflorus* on the viability of human prostate cancer PC3 Cells: PC3 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in 'Material and Methods', and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human prostate cancer LNCap cells



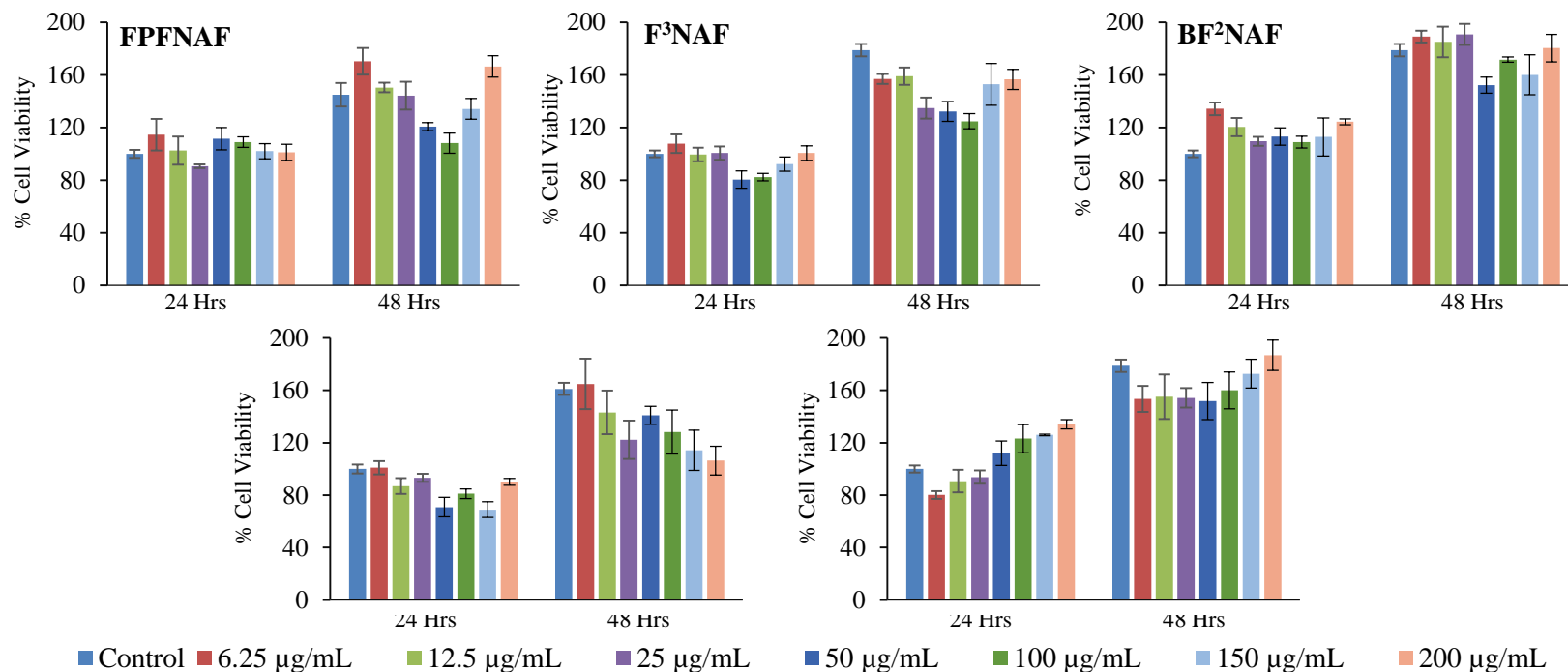
**Figure.** Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human prostate cancer LNCap cells: LNCap cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in ‘Material and Methods’, and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human prostate cancer LNCap cells



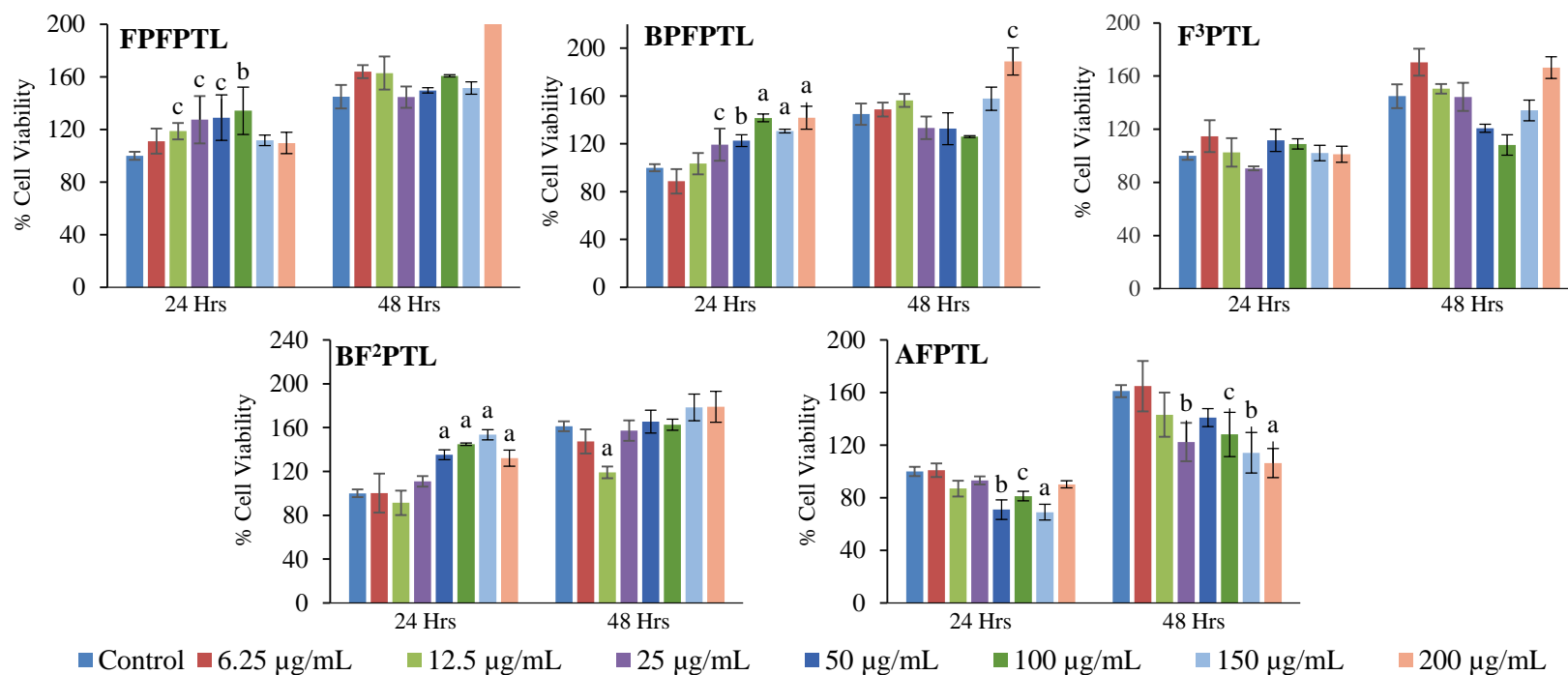
**Figure.** Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human prostate cancer LNCap cells: LNCap cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in ‘Material and Methods’, and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human colon cancer SW480 cells



**Figure.** Effects of different fractions of *Nyctanthes arbor-tristis* on the viability of human colon cancer SW480 cells: SW480 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in ‘Material and Methods’, and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human colon cancer SW480 cells



**Figure.** Effects of different fractions of *Phlogacanthus thyrsoiflorus* on the viability of human colon cancer SW480 cells: SW480 cells treated with various concentration of fractions in DMSO for 24-48 hrs. At the end of each treatment duration, viability was measured by MTT assay as mentioned in 'Material and Methods', and % cell viability are shown. The values are represented as mean  $\pm$  SEM of three samples for each treatment. c,  $P < 0.05$ ; b,  $P < 0.01$ ; a,  $P < 0.001$ .

## Qualitative Compound Report

**Data File** F3NAF.d **Sample Name** F3NAF  
**Sample Type** Sample **Position** P1-A1  
**Instrument Name** Instrument 1 **User Name**  
**Acq Method** 30mins\_+ESI\_10032014.m **Acquired Time** 1/6/2016 4:14:38 PM  
**IRM Calibration Status** Success **DA Method** default.m  
**Comment**

**Sample Group** Info.  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.05.01 (B5125.1)

## Compound Table

| Compound Label   | RT    | Mass     | Name   | Formula         | MFG Formula     | DB Formula      | DB Diff (ppm) | Hits (DB) |
|--|-------|----------|--|-----------------|-----------------|-----------------|---------------|-----------|
| Cpd 1: isoamyl nitrite   | 0.505 | 117.0783 | isoamyl nitrite  | C5 H11 N O2     | C5 H11 N O2     | C5 H11 N O2     | 5.67          | 8         |
| Cpd 2: 0.509   | 0.509 | 101.12   |  |                 |                 |                 |               |           |
| Cpd 3: Methyl N-(a-methylbutyl)glycine   | 0.514 | 173.1047 | Methyl N-(a-methylbutyl)glycine  | C8 H15 N O3     | C8 H15 N O3     | C8 H15 N O3     | 2.73          | 13        |
| Cpd 4: Nefopam   | 0.523 | 253.1519 | Nefopam  | C17 H19 N O     | C17 H19 N O     | C17 H19 N O     | -20.54        | 1         |
| Cpd 5: 2-Aminomuconate 6-semialdehyde  | 0.546 | 141.0422 | 2-Aminomuconate 6-semialdehyde   | O6 H7 N O3      | O6 H7 N O3      | O6 H7 N O3      | 2.78          | 12        |
| Cpd 6: 2-Aminomuconate 6-semialdehyde  | 0.674 | 141.0423 | 2-Aminomuconate 6-semialdehyde   | O6 H7 N O3      | O6 H7 N O3      | O6 H7 N O3      | 2.32          | 12        |
| Cpd 7: 1-Methyl-5-imidazoleacetic acid   | 0.675 | 140.0582 | 1-Methyl-5-imidazoleacetic acid  | O6 H8 N2 O2     | O6 H8 N2 O2     | O6 H8 N2 O2     | 3.03          | 6         |
| Cpd 8: 1-(3-Carboxypropyl)-3,7-dimethylxanthine  | 0.747 | 266.0996 | 1-(3-Carboxypropyl)-3,7-dimethylxanthine   | C11 H14 N4 O4   | C11 H14 N4 O4   | C11 H14 N4 O4   | 7.3           | 5         |
| Cpd 9: 2-octynoic acid   | 0.975 | 140.0832 | 2-octynoic acid  | C8 H12 O2       | C8 H12 O2       | C8 H12 O2       | 3.91          | 12        |
| Cpd 10: Shikimic acid  | 3.081 | 174.0523 | Shikimic acid  | C7 H10 O5       | C7 H10 O5       | C7 H10 O5       | 3.2           | 12        |
| Cpd 11: Ethyl Oxalacetate  | 3.874 | 188.068  | Ethyl Oxalacetate  | C8 H12 O5       | C8 H12 O5       | C8 H12 O5       | 2.71          | 4         |
| Cpd 12: Asn Ala Cys  | 3.906 | 306.0945 | Asn Ala Cys  | C10 H18 N4 O5 S | C10 H18 N4 O5 S | C10 H18 N4 O5 S | 17.36         | 12        |
| Cpd 13: 2-Furanpropionic acid, tetrahydro-a-(1-naphthylmethyl)-  | 3.984 | 284.1459 | 2-Furanpropionic acid, tetrahydro-a-(1-naphthylmethyl)-  | C18 H20 O3      | C18 H20 O3      | C18 H20 O3      | -16.34        | 4         |
| Cpd 14: 4-Hydroxylevamisole Glucuronide  | 4.539 | 396.102  | 4-Hydroxylevamisole Glucuronide  | C17 H20 N2 O7 S | C17 H20 N2 O7 S | C17 H20 N2 O7 S | -7.18         | 14        |
| Cpd 15: 6-propionyl n-caproic acid   | 4.707 | 172.1094 | 6-propionyl n-caproic acid   | C9 H16 O3       | C9 H16 O3       | C9 H16 O3       | 3.06          | 15        |
| Cpd 16: Methyl o-methoxyhippuric acid  | 4.996 | 223.0838 | Methyl o-methoxyhippuric acid  | C11 H13 N O4    | C11 H13 N O4    | C11 H13 N O4    | 2.79          | 13        |
| Cpd 17: Quinol glucuronide   | 5.022 | 286.0675 | Quinol glucuronide   | C12 H14 O8      | C12 H14 O8      | C12 H14 O8      | 4.63          | 3         |
| Cpd 18: 9-hydroxy-2E-decenoic acid   | 5.032 | 186.125  | 9-hydroxy-2E-decenoic acid   | C10 H18 O3      | C10 H18 O3      | C10 H18 O3      | 3.14          | 15        |
| Cpd 19: Methyl o-methoxyhippuric acid  | 5.083 | 223.0839 | Methyl o-methoxyhippuric acid  | C11 H13 N O4    | C11 H13 N O4    | C11 H13 N O4    | 2.72          | 8         |
| Cpd 20: Phe His  | 5.376 | 302.1356 | Phe His  | C15 H18 N4 O3   | C15 H18 N4 O3   | C15 H18 N4 O3   | 7.43          | 2         |
| Cpd 21: Ibuprofen  | 5.414 | 206.1302 | Ibuprofen  | C13 H18 O2      | C13 H18 O2      | C13 H18 O2      | 2.16          | 15        |
| Cpd 22: Methyl jasmonate   | 5.422 | 224.1406 | Methyl jasmonate   | C13 H20 O3      | C13 H20 O3      | C13 H20 O3      | 2.77          | 15        |
| Cpd 23: Benzenemethanol, 2-(2-aminopropoxy)-3-methyl-  | 5.799 | 196.1094 | Benzenemethanol, 2-(2-aminopropoxy)-3-methyl-  | C11 H16 O3      | C11 H16 O3      | C11 H16 O3      | 2.61          | 2         |
| Cpd 24: Isovaleric acid  | 5.878 | 102.0676 | Isovaleric acid  | C5 H10 O2       | C5 H10 O2       | C5 H10 O2       | 4.21          | 5         |
| Cpd 25: 2E,7E-decadienoic acid   | 5.878 | 168.1145 | 2E,7E-decadienoic acid   | C10 H16 O2      | C10 H16 O2      | C10 H16 O2      | 3.13          | 15        |
| Cpd 26: 4-octenal  | 5.878 | 126.104  | 4-octenal  | C8 H14 O        | C8 H14 O        | C8 H14 O        | 3.9           | 7         |
| Cpd 27: 2-nonenal  | 5.878 | 140.1196 | 2-nonenal  | C9 H16 O        | C9 H16 O        | C9 H16 O        | 3.89          | 5         |
| Cpd 28: beta-nonylenic acid  | 5.879 | 156.1144 | beta-nonylenic acid  | C9 H16 O2       | C9 H16 O2       | C9 H16 O2       | 4.01          | 15        |
| Cpd 29: 9-hydroxy-2E-decenoic acid   | 5.893 | 186.125  | 9-hydroxy-2E-decenoic acid   | C10 H18 O3      | C10 H18 O3      | C10 H18 O3      | 3.39          | 15        |
| Cpd 30: ((2R)-1alpha,22,25-trihydroxy-26,27-dimethyl-23,24-tetrahydro-24a-homo-20-epivitamin D3 / (22R)-1a | 5.897 | 470.3445 | ((2R)-1alpha,22,25-trihydroxy-26,27-dimethyl-23,24-tetrahydro-24a-homo-20-epivitamin D3 / (22R)-1a | C30 H46 O4      | C30 H46 O4      | C30 H46 O4      | -10.49        | 15        |
| Cpd 31: Hydroxyibuprofen   | 6.016 | 222.1251 | Hydroxyibuprofen   | C13 H18 O3      | C13 H18 O3      | C13 H18 O3      | 2.03          | 15        |
| Cpd 32: Hydroxyibuprofen   | 6.019 | 222.125  | Hydroxyibuprofen   | C13 H18 O3      | C13 H18 O3      | C13 H18 O3      | 2.8           | 10        |
| Cpd 33: Benzenemethanol, 2-(2-aminopropoxy)-3-methyl-  | 6.072 | 196.1095 | Benzenemethanol, 2-(2-aminopropoxy)-3-methyl-  | C11 H16 O3      | C11 H16 O3      | C11 H16 O3      | 2.09          | 2         |
| Cpd 34: 6.109  | 6.109 | 565.418  |  |                 |                 |                 |               |           |
| Cpd 35: 4-(2-hydroxypropoxy)-3,5-dimethyl-Phenol   | 6.203 | 196.1094 | 4-(2-hydroxypropoxy)-3,5-dimethyl-Phenol   | C11 H16 O3      | C11 H16 O3      | C11 H16 O3      | 2.56          | 10        |
| Cpd 36: LOGANIC ACID   | 6.386 | 376.1352 | LOGANIC ACID   | C16 H24 O10     | C16 H24 O10     | C16 H24 O10     | 4.63          | 15        |
| Cpd 37: Methyl jasmonate   | 6.627 | 224.1407 | Methyl jasmonate   | C13 H20 O3      | C13 H20 O3      | C13 H20 O3      | 2.58          | 15        |
| Cpd 38: Citronellic acid   | 6.96  | 170.1301 | Citronellic acid   | C10 H18 O2      | C10 H18 O2      | C10 H18 O2      | 3.19          | 15        |
| Cpd 39: Mitoxantrone   | 7     | 444.1975 | Mitoxantrone   | C22 H28 N4 O6   | C22 H28 N4 O6   | C22 H28 N4 O6   | 7.59          | 12        |
| Cpd 40: Acetylsalicylic acid (aspirin)   | 7.036 | 180.0418 | Acetylsalicylic acid (aspirin)   | C9 H8 O4        | C9 H8 O4        | C9 H8 O4        | 2.71          | 14        |
| Cpd 41: Gln Gln Asn  | 7.076 | 388.1718 | Gln Gln Asn  | C14 H24 N6 O7   | C14 H24 N6 O7   | C14 H24 N6 O7   | -3.04         | 15        |
| Cpd 42: Ubiquinone   | 7.077 | 250.1199 | Ubiquinone   | C14 H18 O4      | C14 H18 O4      | C14 H18 O4      | 2.33          | 4         |
| Cpd 43: Phe Tyr Gln  | 7.141 | 456.1978 | Phe Tyr Gln  | C23 H28 N4 O6   | C23 H28 N4 O6   | C23 H28 N4 O6   | 6.8           | 15        |
| Cpd 44: Deutioside   | 7.189 | 346.125  | Deutioside   | C15 H22 O9      | C15 H22 O9      | C15 H22 O9      | 3.88          | 15        |
| Cpd 45: PGD2   | 7.282 | 352.2235 | PGD2   | C20 H32 O5      | C20 H32 O5      | C20 H32 O5      | 4.23          | 15        |
| Cpd 46: Ubiquinone   | 7.285 | 250.1199 | Ubiquinone   | C14 H18 O4      | C14 H18 O4      | C14 H18 O4      | 2.56          | 4         |
| Cpd 47: Gln Gln Asn  | 7.287 | 388.172  | Gln Gln Asn  | C14 H24 N6 O7   | C14 H24 N6 O7   | C14 H24 N6 O7   | -3.61         | 15        |
| Cpd 48: Penicilloic acid V   | 7.314 | 368.1071 | Penicilloic acid V   | C16 H20 N2 O6 S | C16 H20 N2 O6 S | C16 H20 N2 O6 S | -7.74         | 10        |



## Qualitative Compound Report

|   |       |          |   |                  |                  |                  |        |    |
|---|-------|----------|---|------------------|------------------|------------------|--------|----|
| Cpd 49: Nerolidyl diphosphate   | 7.348 | 382.1247 | Nerolidyl diphosphate   | C15 H28 O7 P2    | C15 H28 O7 P2    | C15 H28 O7 P2    | 16.54  | 15 |
| Cpd 50: Phenylmethyl methyl ketone  | 7.414 | 134.0725 | Phenylmethyl methyl ketone  | C9 H10 O         | C9 H10 O         | C9 H10 O         | 4.93   | 15 |
| Cpd 51: Ginkgolide B  | 7.509 | 424.1355 | Ginkgolide B  | C20 H24 O10      | C20 H24 O10      | C20 H24 O10      | 3.41   | 5  |
| Cpd 52: Penicilloic acid V  | 7.566 | 368.1073 | Penicilloic acid V  | C16 H20 N2 O6 S  | C16 H20 N2 O6 S  | C16 H20 N2 O6 S  | -8.42  | 10 |
| Cpd 53: 2-Keto-3-deoxyoctonate (KDO)  | 7.567 | 238.0683 | 2-Keto-3-deoxyoctonate (KDO)  | C8 H14 O8        | C8 H14 O8        | C8 H14 O8        | 2.24   | 5  |
| Cpd 54: m-Cresol  | 7.567 | 108.0571 | m-Cresol  | C7 H8 O          | C7 H8 O          | C7 H8 O          | 4.17   | 5  |
| Cpd 55: His Ser Val   | 7.568 | 341.1694 | His Ser Val   | C14 H23 N5 O5    | C14 H23 N5 O5    | C14 H23 N5 O5    | 1.4    | 15 |
| Cpd 56: Hydroxyibuprofen  | 7.812 | 222.1255 | Hydroxyibuprofen  | C13 H18 O3       | C13 H18 O3       | C13 H18 O3       | 2.51   | 15 |
| Cpd 57: 3-Phenoxypropionic acid   | 7.812 | 166.0627 | 3-Phenoxypropionic acid   | C9 H10 O3        | C9 H10 O3        | C9 H10 O3        | 1.67   | 15 |
| Cpd 58: Tyr Gln Tyr   | 7.856 | 472.1927 | Tyr Gln Tyr   | C23 H28 N4 O7    | C23 H28 N4 O7    | C23 H28 N4 O7    | 6.46   | 15 |
| Cpd 59: PHENETHICILLIN  | 7.951 | 364.1147 | PHENETHICILLIN  | C17 H20 N2 O5 S  | C17 H20 N2 O5 S  | C17 H20 N2 O5 S  | -14.98 | 9  |
| Cpd 60: 7.951   | 7.951 | 750.2109 |   |                  |                  |                  |        |    |
| Cpd 61: Nerolidyl diphosphate   | 7.953 | 382.1249 | Nerolidyl diphosphate   | C15 H28 O7 P2    | C15 H28 O7 P2    | C15 H28 O7 P2    | 15.97  | 15 |
| Cpd 62: Methyl jasmonate  | 8.027 | 224.1407 | Methyl jasmonate  | C13 H20 O3       | C13 H20 O3       | C13 H20 O3       | 2.5    | 15 |
| Cpd 63: 4,10-undecadienal   | 8.035 | 162.1037 | 4,10-undecadienal   | C11 H14 O        | C11 H14 O        | C11 H14 O        | 4.44   | 15 |
| Cpd 64: 4-Ethylbenzoic acid   | 8.062 | 150.0676 | 4-Ethylbenzoic acid   | C9 H10 O2        | C9 H10 O2        | C9 H10 O2        | 3.43   | 10 |
| Cpd 65: 2-Hydroxy-3-(4-methoxyethylphenoxy)-propanoic acid                  | 8.067 | 240.0992 | 2-Hydroxy-3-(4-methoxyethylphenoxy)-propanoic acid                  | C12 H16 O5       | C12 H16 O5       | C12 H16 O5       | 2.3    | 12 |
| Cpd 66: Asn Asn Asn   | 8.067 | 360.1412 | Asn Asn Asn   | C12 H20 N6 O7    | C12 H20 N6 O7    | C12 H20 N6 O7    | -5.09  | 15 |
| Cpd 67: Val Thr His   | 8.067 | 355.1851 | Val Thr His   | C15 H25 N5 O5    | C15 H25 N5 O5    | C15 H25 N5 O5    | 1.26   | 15 |
| Cpd 68: Acetylsalicylic acid (aspirin)                                      | 8.074 | 180.0417 | Acetylsalicylic acid (aspirin)                                      | C9 H8 O4         | C9 H8 O4         | C9 H8 O4         | 2.99   | 14 |
| Cpd 69: Met Asn Gly   | 8.074 | 320.1121 | Met Asn Gly   | C11 H20 N4 O5 S  | C11 H20 N4 O5 S  | C11 H20 N4 O5 S  | 10.4   | 14 |
| Cpd 70: Met Trp Glu   | 8.076 | 464.1667 | Met Trp Glu   | C21 H28 N4 O6 S  | C21 H28 N4 O6 S  | C21 H28 N4 O6 S  | 13.38  | 6  |
| Cpd 71: 8.096   | 8.096 | 236.1406 |   |                  |                  |                  |        |    |
| Cpd 72: Mitoxantrone  | 8.152 | 444.1978 | Mitoxantrone  | C22 H28 N4 O6    | C22 H28 N4 O6    | C22 H28 N4 O6    | 7      | 12 |
| Cpd 73: Farnesyl pyrophosphate  | 8.176 | 382.1252 | Farnesyl pyrophosphate  | C15 H28 O7 P2    | C15 H28 O7 P2    | C15 H28 O7 P2    | 15.17  | 15 |
| Cpd 74: 2-Hydroxy-3-(4-methoxyethylphenoxy)-propanoic acid                  | 8.354 | 240.0993 | 2-Hydroxy-3-(4-methoxyethylphenoxy)-propanoic acid                  | C12 H16 O5       | C12 H16 O5       | C12 H16 O5       | 2.14   | 12 |
| Cpd 75: 2-Keto-3-deoxyoctonate (KDO)  | 8.354 | 238.0683 | 2-Keto-3-deoxyoctonate (KDO)  | C8 H14 O8        | C8 H14 O8        | C8 H14 O8        | 2.45   | 6  |
| Cpd 76: 4-Ethylbenzoic acid   | 8.354 | 150.0675 | 4-Ethylbenzoic acid   | C9 H10 O2        | C9 H10 O2        | C9 H10 O2        | 3.57   | 15 |
| Cpd 77: Asn Asn Asn   | 8.355 | 360.1408 | Asn Asn Asn   | C12 H20 N6 O7    | C12 H20 N6 O7    | C12 H20 N6 O7    | -4.16  | 15 |
| Cpd 78: Val Thr His   | 8.355 | 355.1853 | Val Thr His   | C15 H25 N5 O5    | C15 H25 N5 O5    | C15 H25 N5 O5    | 0.76   | 15 |
| Cpd 79: Phenylmethyl methyl ketone  | 8.355 | 134.0725 | Phenylmethyl methyl ketone  | C9 H10 O         | C9 H10 O         | C9 H10 O         | 5.03   | 6  |
| Cpd 80: Desmethylnaproxen-6-O-glucuronide                                   | 8.409 | 392.1095 | Desmethylnaproxen-6-O-glucuronide                                   | C19 H20 O9       | C19 H20 O9       | C19 H20 O9       | 3.25   | 10 |
| Cpd 81: 1-Methyl-4-nitro-5-(S-Glutathionyl) Imidazole                       | 8.416 | 432.1047 | 1-Methyl-4-nitro-5-(S-Glutathionyl) Imidazole                       | C14 H20 N6 O8 S  | C14 H20 N6 O8 S  | C14 H20 N6 O8 S  | 3.84   | 7  |
| Cpd 82: alpha-Erythroidine  | 8.429 | 273.1359 | alpha-Erythroidine  | C16 H19 N O3     | C16 H19 N O3     | C16 H19 N O3     | 2.3    | 14 |
| Cpd 83: Fluocinolone  | 8.45  | 412.1697 | Fluocinolone  | C21 H26 F2 O6    | C21 H26 F2 O6    | C21 H26 F2 O6    | 0.13   | 15 |
| Cpd 84: Ginkgolide A  | 8.5   | 408.1405 | Ginkgolide A  | C20 H24 O9       | C20 H24 O9       | C20 H24 O9       | 3.67   | 15 |
| Cpd 85: 8.500   | 8.5   | 552.1823 |   |                  |                  |                  |        |    |
| Cpd 86: 8.590   | 8.59  | 584.1719 |   |                  |                  |                  |        |    |
| Cpd 87: Fluocinolone  | 8.64  | 412.1693 | Fluocinolone  | C21 H26 F2 O6    | C21 H26 F2 O6    | C21 H26 F2 O6    | 1.12   | 15 |
| Cpd 88: Salicin   | 8.668 | 286.1067 | Salicin   | C13 H18 O7       | C13 H18 O7       | C13 H18 O7       | -5.08  | 6  |
| Cpd 89: Phenylpyruvic acid  | 8.67  | 164.047  | Phenylpyruvic acid  | C9 H8 O3         | C9 H8 O3         | C9 H8 O3         | 2.16   | 15 |
| Cpd 90: Cys Trp Tyr   | 8.676 | 470.1539 | Cys Trp Tyr   | C23 H26 N4 O5 S  | C23 H26 N4 O5 S  | C23 H26 N4 O5 S  | 17.99  | 6  |
| Cpd 91: Lys Glu Lys   | 8.751 | 403.2427 | Lys Glu Lys   | C17 H33 N5 O6    | C17 H33 N5 O6    | C17 H33 N5 O6    | 1      | 15 |
| Cpd 92: Fluocinolone  | 8.751 | 412.1695 | Fluocinolone  | C21 H26 F2 O6    | C21 H26 F2 O6    | C21 H26 F2 O6    | 0.68   | 15 |
| Cpd 93: a-N-Acetylneuraminy-2,6-b-D-galactosyl-1,4-N-acetyl-b-D-glucosamine | 8.838 | 674.2525 | a-N-Acetylneuraminy-2,6-b-D-galactosyl-1,4-N-acetyl-b-D-glucosamine | C25 H42 N2 O19   | C25 H42 N2 O19   | C25 H42 N2 O19   | -21.18 | 1  |
| Cpd 94: 8.872   | 8.872 | 554.2107 |   |                  |                  |                  |        |    |
| Cpd 95: Ginkgolide A  | 8.994 | 408.139  | Ginkgolide A  | C20 H24 O9       | C20 H24 O9       | C20 H24 O9       | 7.32   | 15 |
| Cpd 96: CLOVANEDIOL DIACETATE   | 9.017 | 322.2134 | CLOVANEDIOL DIACETATE   | C19 H30 O4       | C19 H30 O4       | C19 H30 O4       | 3.04   | 15 |
| Cpd 97: Desmethylnaproxen-6-O-glucuronide                                   | 9.188 | 392.11   | Desmethylnaproxen-6-O-glucuronide                                   | C19 H20 O9       | C19 H20 O9       | C19 H20 O9       | 1.84   | 3  |
| Cpd 98: Desmethylnaproxen-6-O-glucuronide                                   | 9.191 | 392.1095 | Desmethylnaproxen-6-O-glucuronide                                   | C19 H20 O9       | C19 H20 O9       | C19 H20 O9       | 3.02   | 9  |
| Cpd 99: His Glu Gln   | 9.307 | 412.174  | His Glu Gln   | C16 H24 N6 O7    | C16 H24 N6 O7    | C16 H24 N6 O7    | -8.26  | 15 |
| Cpd 100: 9.308  | 9.308 | 578.198  |   |                  |                  |                  |        |    |
| Cpd 101: 9.309  | 9.309 | 595.2241 |   |                  |                  |                  |        |    |
| Cpd 102: N-Didesethylquinagolide sulfate                                    | 9.396 | 419.1207 | N-Didesethylquinagolide sulfate                                     | C16 H25 N3 O6 S2 | C16 H25 N3 O6 S2 | C16 H25 N3 O6 S2 | -5.4   | 15 |
| Cpd 103: Dihydrodeoxystreptomycin   | 9.401 | 567.2872 | Dihydrodeoxystreptomycin  | C21 H41 N7 O11   | C21 H41 N7 O11   | C21 H41 N7 O11   | -1.33  | 4  |
| Cpd 104: SWIETENINE   | 9.401 | 568.2705 | SWIETENINE  | C32 H40 O9       | C32 H40 O9       | C32 H40 O9       | -5.71  | 3  |
| Cpd 105: Fenoprofen glucuronide   | 9.479 | 418.1254 | Fenoprofen glucuronide  | C21 H22 O9       | C21 H22 O9       | C21 H22 O9       | 2.35   | 9  |
| Cpd 106: Phloridzin   | 9.481 | 436.1356 | Phloridzin  | C21 H24 O10      | C21 H24 O10      | C21 H24 O10      | 3.09   | 10 |
| Cpd 107: 2E,7E-decadienoic acid   | 9.582 | 168.1144 | 2E,7E-decadienoic acid  | C10 H16 O2       | C10 H16 O2       | C10 H16 O2       | 3.7    | 15 |
| Cpd 108: 16-hydroxy-5-hexadecenoic acid                                     | 9.609 | 270.2187 | 16-hydroxy-5-hexadecenoic acid                                      | C16 H30 O3       | C16 H30 O3       | C16 H30 O3       | 2.97   | 15 |

## Qualitative Compound Report

|   |        |          |  |                 |                 |                 |       |    |
|---|--------|----------|--|-----------------|-----------------|-----------------|-------|----|
| Cpd 109: 10Z,12E-hexadecadienoic acid   | 9.61   | 252.2082 | 10Z,12E-hexadecadienoic acid   | C16 H28 O2      | C16 H28 O2      | C16 H28 O2      | 2.72  | 15 |
| Cpd 110: 9.650  | 9.65   | 180.1145 |  |                 |                 |                 |       |    |
| Cpd 111: Neu5Gcalpha2-3Galbeta1-4Gcbeta-Sp  | 9.685  | 718.2215 | Neu5Gcalpha2-3Galbeta1-4Gcbeta-Sp  | C25 H42 N4 O20  | C25 H42 N4 O20  | C25 H42 N4 O20  | 24.77 | 1  |
| Cpd 112: Torasemide   | 9.685  | 348.1198 | Torasemide   | C16 H20 N4 O3 S | C16 H20 N4 O3 S | C16 H20 N4 O3 S | 16.6  | 15 |
| Cpd 113: 9.742  | 9.742  | 670.1875 |  |                 |                 |                 |       |    |
| Cpd 114: 9.785  | 9.785  | 568.1769 |  |                 |                 |                 |       |    |
| Cpd 115: Hexadecanedioic acid   | 10.011 | 286.2136 | Hexadecanedioic acid   | C16 H30 O4      | C16 H30 O4      | C16 H30 O4      | 2.91  | 6  |
| Cpd 116: (24R)-25-fluoro-1alpha,24-dihydroxy-24-methylvitamin D3 / (24R)-25-fluoro-1alpha,24-dihydroxy-24-met | 10.058 | 448.3383 | (24R)-25-fluoro-1alpha,24-dihydroxy-24-methylvitamin D3 / (24R)-25-fluoro-1alpha,24-dihydroxy-24-met | C28 H45 F O3    | C28 H45 F O3    | C28 H45 F O3    | -6.7  | 2  |
| Cpd 117: 4-Ketoretinoic acid glucuronide  | 10.148 | 490.2207 | 4-Ketoretinoic acid glucuronide  | C26 H34 O9      | C26 H34 O9      | C26 H34 O9      | -0.88 | 5  |
| Cpd 118: Tyr Trp Tyr  | 10.151 | 530.2133 | Tyr Trp Tyr  | C29 H30 N4 O6   | C29 H30 N4 O6   | C29 H30 N4 O6   | 6.1   | 6  |
| Cpd 119: Phloridzin   | 10.18  | 436.1352 | Phloridzin   | C21 H24 O10     | C21 H24 O10     | C21 H24 O10     | 4.02  | 9  |
| Cpd 120: Terazosin  | 10.271 | 387.1902 | Terazosin  | C19 H25 N5 O4   | C19 H25 N5 O4   | C19 H25 N5 O4   | 1.17  | 15 |
| Cpd 121: 2,3-Dinor-6,15-diketo-13,14-dihydro-20-carboxyl-PGF1a  | 10.274 | 370.1634 | 2,3-Dinor-6,15-diketo-13,14-dihydro-20-carboxyl-PGF1a  | C18 H26 O8      | C18 H26 O8      | C18 H26 O8      | -1.81 | 15 |
| Cpd 122: Elephantopin   | 10.276 | 360.1196 | Elephantopin   | C19 H20 O7      | C19 H20 O7      | C19 H20 O7      | 3.55  | 15 |
| Cpd 123: b-D-Glucopyranosiduronic acid, 6-(3-hydroxybutyl)-2-naphthalenyl                                     | 10.286 | 392.1463 | b-D-Glucopyranosiduronic acid, 6-(3-hydroxybutyl)-2-naphthalenyl                                     | C20 H24 O8      | C20 H24 O8      | C20 H24 O8      | 2.13  | 15 |
| Cpd 124: (24R)-25-fluoro-1alpha,24-dihydroxy-24-methylvitamin D3 / (24R)-25-fluoro-1alpha,24-dihydroxy-24-met | 10.316 | 448.3383 | (24R)-25-fluoro-1alpha,24-dihydroxy-24-methylvitamin D3 / (24R)-25-fluoro-1alpha,24-dihydroxy-24-met | C28 H45 F O3    | C28 H45 F O3    | C28 H45 F O3    | -6.78 | 2  |
| Cpd 125: Trandolaprilat glucuronide   | 10.371 | 578.2345 | Trandolaprilat glucuronide   | C28 H38 N2 O11  | C28 H38 N2 O11  | C28 H38 N2 O11  | 22.6  | 1  |
| Cpd 126: 2,3-Dinor-6,15-diketo-13,14-dihydro-20-carboxyl-PGF1a  | 10.456 | 370.1634 | 2,3-Dinor-6,15-diketo-13,14-dihydro-20-carboxyl-PGF1a  | C18 H26 O8      | C18 H26 O8      | C18 H26 O8      | -1.67 | 15 |
| Cpd 127: Terazosin  | 10.456 | 387.1901 | Terazosin  | C19 H25 N5 O4   | C19 H25 N5 O4   | C19 H25 N5 O4   | 1.45  | 15 |
| Cpd 128: MYCOPHENOLIC ACID  | 10.456 | 320.1271 | MYCOPHENOLIC ACID  | C17 H20 O6      | C17 H20 O6      | C17 H20 O6      | -3.44 | 15 |
| Cpd 129: b-D-Glucopyranosiduronic acid, 6-(3-hydroxybutyl)-2-naphthalenyl                                     | 10.457 | 392.1461 | b-D-Glucopyranosiduronic acid, 6-(3-hydroxybutyl)-2-naphthalenyl                                     | C20 H24 O8      | C20 H24 O8      | C20 H24 O8      | 2.72  | 15 |
| Cpd 130: 4-oxo-9Z,11Z,13E,15E-octadecatetraenoic acid   | 10.483 | 290.1871 | 4-oxo-9Z,11Z,13E,15E-octadecatetraenoic acid   | C18 H26 O3      | C18 H26 O3      | C18 H26 O3      | 3.85  | 13 |
| Cpd 131: ACECLIDINE   | 10.56  | 169.11   | ACECLIDINE   | C9 H15 N O2     | C9 H15 N O2     | C9 H15 N O2     | 1.74  | 10 |
| Cpd 132: Pro Thr Trp  | 10.56  | 402.1926 | Pro Thr Trp  | C20 H26 N4 O5   | C20 H26 N4 O5   | C20 H26 N4 O5   | -5.59 | 15 |
| Cpd 133: 7-[2-TRIFLUOROMETHYL-4-(2-HYDROXYPHENYL)-1,3-DIOXAN-cis-5-YL]-HEPT-5Z-ENOIC ACID                     | 10.64  | 374.1949 | 7-[2-TRIFLUOROMETHYL-4-(2-HYDROXYPHENYL)-1,3-DIOXAN-cis-5-YL]-HEPT-5Z-ENOIC ACID                     | C18 H21 F3 O5   | C18 H21 F3 O5   | C18 H21 F3 O5   | -2.05 | 15 |
| Cpd 134: gamma-Hydroxyphenylbutazone glucuronide  | 10.696 | 500.1689 | gamma-Hydroxyphenylbutazone glucuronide  | C25 H28 N2 O9   | C25 H28 N2 O9   | C25 H28 N2 O9   | 21.15 | 2  |
| Cpd 135: 10.698   | 10.698 | 684.2029 |  |                 |                 |                 |       |    |
| Cpd 136: QUERCETIN TETRAMETHYL (5,7,3',4') ETHER  | 10.76  | 358.1035 | QUERCETIN TETRAMETHYL (5,7,3',4') ETHER  | C19 H18 O7      | C19 H18 O7      | C19 H18 O7      | 5.01  | 12 |
| Cpd 137: Ginkgolide A   | 10.763 | 408.1407 | Ginkgolide A   | C20 H24 O9      | C20 H24 O9      | C20 H24 O9      | 3.17  | 15 |
| Cpd 138: 4-Methoxycinnamic acid   | 10.797 | 178.0627 | 4-Methoxycinnamic acid   | C10 H10 O3      | C10 H10 O3      | C10 H10 O3      | 1.81  | 9  |
| Cpd 139: 10.797   | 10.797 | 670.2239 |  |                 |                 |                 |       |    |
| Cpd 140: 10.836   | 10.836 | 256.084  |  |                 |                 |                 |       |    |
| Cpd 141: XYLOCARPUS A   | 11.173 | 586.2392 | XYLOCARPUS A   | C31 H38 O11     | C31 H38 O11     | C31 H38 O11     | 3.78  | 2  |
| Cpd 142: Ile Trp Asn  | 11.247 | 431.2165 | Ile Trp Asn  | C21 H29 N5 O5   | C21 H29 N5 O5   | C21 H29 N5 O5   | 0.94  | 15 |
| Cpd 143: Thr Cys Arg  | 11.25  | 378.1688 | Thr Cys Arg  | C13 H26 N6 O5 S | C13 H26 N6 O5 S | C13 H26 N6 O5 S | -0.74 | 15 |
| Cpd 144: Gibberellin A8   | 11.253 | 364.1534 | Gibberellin A8   | C19 H24 O7      | C19 H24 O7      | C19 H24 O7      | -3.19 | 15 |
| Cpd 145: TRIPTONIDE   | 11.254 | 358.1403 | TRIPTONIDE   | C20 H22 O6      | C20 H22 O6      | C20 H22 O6      | 3.64  | 15 |
| Cpd 146: Thr Trp Met  | 11.258 | 436.1712 | Thr Trp Met  | C20 H28 N4 O5 S | C20 H28 N4 O5 S | C20 H28 N4 O5 S | 15.72 | 6  |
| Cpd 147: Folic acid   | 11.42  | 441.1407 | Folic acid   | C19 H19 N7 O6   | C19 H19 N7 O6   | C19 H19 N7 O6   | -2.23 | 1  |
| Cpd 148: Ile Trp Asn  | 11.449 | 431.2162 | Ile Trp Asn  | C21 H29 N5 O5   | C21 H29 N5 O5   | C21 H29 N5 O5   | 1.55  | 15 |
| Cpd 149: Thr Cys Arg  | 11.449 | 378.1688 | Thr Cys Arg  | C13 H26 N6 O5 S | C13 H26 N6 O5 S | C13 H26 N6 O5 S | -0.75 | 15 |
| Cpd 150: 11.449   | 11.449 | 858.3046 |  |                 |                 |                 |       |    |
| Cpd 151: Gibberellin A8   | 11.449 | 364.1524 | Gibberellin A8   | C19 H24 O7      | C19 H24 O7      | C19 H24 O7      | -0.55 | 15 |
| Cpd 152: Thr Trp Met  | 11.449 | 436.1718 | Thr Trp Met  | C20 H28 N4 O5 S | C20 H28 N4 O5 S | C20 H28 N4 O5 S | 14.35 | 7  |
| Cpd 153: p-HYDROXYCINNAMALDEHYDE  | 11.45  | 148.0519 | p-HYDROXYCINNAMALDEHYDE  | C9 H8 O2        | C9 H8 O2        | C9 H8 O2        | 3.41  | 11 |
| Cpd 154: 16-hydroxy-5-hexadecenoic acid   | 11.593 | 270.2188 | 16-hydroxy-5-hexadecenoic acid   | C16 H30 O3      | C16 H30 O3      | C16 H30 O3      | 2.48  | 15 |
| Cpd 155: 10Z,12E-hexadecadienoic acid   | 11.595 | 252.2083 | 10Z,12E-hexadecadienoic acid   | C16 H28 O2      | C16 H28 O2      | C16 H28 O2      | 2.37  | 15 |
| Cpd 156: 2-oxo-heptadecanoic acid   | 11.595 | 284.2342 | 2-oxo-heptadecanoic acid   | C17 H32 O3      | C17 H32 O3      | C17 H32 O3      | 3.44  | 7  |
| Cpd 157: Gibberellin A8-catabolite  | 11.664 | 362.1376 | Gibberellin A8-catabolite  | C19 H22 O7      | C19 H22 O7      | C19 H22 O7      | -2.77 | 15 |

## Qualitative Compound Report

|  |        |          |   |                  |                  |                  |        |    |
|--|--------|----------|---|------------------|------------------|------------------|--------|----|
| Cpd 158: Idebenone Metabolite (Benzenedecanoic acid, 2-hydroxy-3,4-dimethoxy-6-methyl-5-(sulfoxy)-)  | 11.665 | 434.1559 | Idebenone Metabolite (Benzenedecanoic acid, 2-hydroxy-3,4-dimethoxy-6-methyl-5-(sulfoxy)-)  | C19 H30 O9 S     | C19 H30 O9 S     | C19 H30 O9 S     | 11.76  | 2  |
| Cpd 159: p-HYDROXYCINNAMALDEHYDE   | 11.68  | 148.0519 | p-HYDROXYCINNAMALDEHYDE   | C9 H8 O2         | C9 H8 O2         | C9 H8 O2         | 3.46   | 11 |
| Cpd 160: 7-[2-TRIFLUOROMETHYL-4-(2-HYDROXYPHENYL)-1,3-DIOXAN-cis-5-YL]-HEPT-5Z-FUNIC ACID  | 11.683 | 374.1351 | 7-[2-TRIFLUOROMETHYL-4-(2-HYDROXYPHENYL)-1,3-DIOXAN-cis-5-YL]-HEPT-5Z-FUNIC ACID  | C18 H21 F3 O5    | C18 H21 F3 O5    | C18 H21 F3 O5    | -2.65  | 15 |
| Cpd 161: 11.801  | 11.801 | 495.151  |   |                  |                  |                  |        |    |
| Cpd 162: Metaproterenol  | 12.137 | 211.1204 | Metaproterenol  | C11 H17 N O3     | C11 H17 N O3     | C11 H17 N O3     | 2.29   | 10 |
| Cpd 163: Mitoxantrone  | 12.137 | 444.2031 | Mitoxantrone  | C22 H28 N4 O6    | C22 H28 N4 O6    | C22 H28 N4 O6    | -4.98  | 2  |
| Cpd 164: Atorvastatin  | 12.454 | 558.2445 | Atorvastatin  | C33 H35 F N2 O5  | C33 H35 F N2 O5  | C33 H35 F N2 O5  | 15.28  | 2  |
| Cpd 165: Mefenamic acid  | 12.554 | 241.1096 | Mefenamic acid  | C15 H15 N O2     | C15 H15 N O2     | C15 H15 N O2     | 2.64   | 11 |
| Cpd 166: Phenylbutazone glucuronide  | 12.553 | 484.1736 | Phenylbutazone glucuronide  | C25 H28 N2 O8    | C25 H28 N2 O8    | C25 H28 N2 O8    | 22.56  | 2  |
| Cpd 167: FLUTRIMAZOLE  | 12.866 | 346.1303 | FLUTRIMAZOLE  | C22 H16 F2 N2    | C22 H16 F2 N2    | C22 H16 F2 N2    | -6.32  | 15 |
| Cpd 168: 13.051  | 13.051 | 522.1507 |   |                  |                  |                  |        |    |
| Cpd 169: Bilirubin   | 13.223 | 584.26   | Bilirubin   | C33 H36 N4 O6    | C33 H36 N4 O6    | C33 H36 N4 O6    | 5.88   | 3  |
| Cpd 170: 4-Methoxycinnamic acid  | 13.389 | 178.0625 | 4-Methoxycinnamic acid  | C10 H10 O3       | C10 H10 O3       | C10 H10 O3       | 2.91   | 9  |
| Cpd 171: 13.403  | 13.403 | 508.1712 |   |                  |                  |                  |        |    |
| Cpd 172: 4-Methoxycinnamic acid  | 13.559 | 178.0625 | 4-Methoxycinnamic acid  | C10 H10 O3       | C10 H10 O3       | C10 H10 O3       | 2.74   | 9  |
| Cpd 173: Nalbuphine-6-sulfate  | 13.758 | 437.1487 | Nalbuphine-6-sulfate  | C21 H27 N O7 S   | C21 H27 N O7 S   | C21 H27 N O7 S   | 4.76   | 2  |
| Cpd 174: 1alpha,25-dihydroxy-26,26,27,27,27-hexafluoro-16,17,23,23,24,24-hexadehydro-19-norvitamin D3 / 1a   | 13.895 | 506.2188 | 1alpha,25-dihydroxy-26,26,27,27,27-hexafluoro-16,17,23,23,24,24-hexadehydro-19-norvitamin D3 / 1a   | C26 H32 F6 O3    | C26 H32 F6 O3    | C26 H32 F6 O3    | 13.37  | 3  |
| Cpd 175: beta-Erythroidine   | 13.895 | 273.1358 | beta-Erythroidine   | C16 H19 N O3     | C16 H19 N O3     | C16 H19 N O3     | 2.35   | 15 |
| Cpd 176: 13.992  | 13.992 | 553.323  |   |                  |                  |                  |        |    |
| Cpd 177: Zopiclone N-oxide   | 14.204 | 404.0913 | Zopiclone N-oxide   | C17 H17 Cl N6 O4 | C17 H17 Cl N6 O4 | C17 H17 Cl N6 O4 | 21.57  | 1  |
| Cpd 178: 14.477  | 14.477 | 495.0673 |   |                  |                  |                  |        |    |
| Cpd 179: Ketotifen-N-glucuronide   | 14.483 | 486.1535 | Ketotifen-N-glucuronide   | C25 H28 N O7 S   | C25 H28 N O7 S   | C25 H28 N O7 S   | 10.56  | 5  |
| Cpd 180: Anandamide (18:3, n-6)  | 14.681 | 321.2654 | Anandamide (18:3, n-6)  | C20 H35 N O2     | C20 H35 N O2     | C20 H35 N O2     | 4.39   | 2  |
| Cpd 181: 14.701  | 14.701 | 555.3381 |   |                  |                  |                  |        |    |
| Cpd 182: Pro Pro Phe   | 14.881 | 359.1842 | Pro Pro Phe   | C19 H25 N3 O4    | C19 H25 N3 O4    | C19 H25 N3 O4    | 0.87   | 15 |
| Cpd 183: (6R)-vitamin D3 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct / (6R)-cholecalciferol 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct / (6R)-cholecalciferol 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct | 15.146 | 559.3696 | (6R)-vitamin D3 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct / (6R)-cholecalciferol 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct / (6R)-cholecalciferol 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct | C35 H49 N3 O3    | C35 H49 N3 O3    | C35 H49 N3 O3    | 13.85  | 2  |
| Cpd 184: GPETn(18:0/18:1(11Z))   | 15.331 | 717.5236 | GPETn(18:0/18:1(11Z))   | C39 H76 N O8 P   | C39 H76 N O8 P   | C39 H76 N O8 P   | 10.16  | 13 |
| Cpd 185: Lactone of PGF-MUM  | 15.334 | 296.1612 | Lactone of PGF-MUM  | C16 H24 O5       | C16 H24 O5       | C16 H24 O5       | 3.99   | 3  |
| Cpd 186: 15.402  | 15.402 | 677.4688 |   |                  |                  |                  |        |    |
| Cpd 187: 15.474  | 15.474 | 633.4425 |   |                  |                  |                  |        |    |
| Cpd 188: GPCho(13:0/10:0[U])   | 15.55  | 608.4347 | GPCho(13:0/10:0[U])   | C31 H63 N O8 P   | C31 H63 N O8 P   | C31 H63 N O8 P   | -9.2   | 13 |
| Cpd 189: GPCho(0-18:0/3:1(2E))   | 15.625 | 564.4087 | GPCho(0-18:0/3:1(2E))   | C29 H59 N O7 P   | C29 H59 N O7 P   | C29 H59 N O7 P   | -10.29 | 2  |
| Cpd 190: 15.701  | 15.701 | 501.3643 |   |                  |                  |                  |        |    |
| Cpd 191: N-Acetylsphingosine   | 15.786 | 341.2915 | N-Acetylsphingosine   | C20 H39 N O3     | C20 H39 N O3     | C20 H39 N O3     | 4.37   | 2  |
| Cpd 192: Phytosphingosine  | 16.557 | 317.2916 | Phytosphingosine  | C18 H39 N O3     | C18 H39 N O3     | C18 H39 N O3     | 4.37   | 7  |
| Cpd 193: 10,16-dihydroxy-palmitic acid   | 17.573 | 288.2312 | 10,16-dihydroxy-palmitic acid   | C16 H32 O4       | C16 H32 O4       | C16 H32 O4       | -3.86  | 15 |
| Cpd 194: 27-nor-5b-cholestane-3a,7a,12a,24,25-pentol   | 18.106 | 438.3321 | 27-nor-5b-cholestane-3a,7a,12a,24,25-pentol   | C26 H46 O5       | C26 H46 O5       | C26 H46 O5       | 5.58   | 1  |
| Cpd 195: 27-nor-5b-cholestane-3a,7a,12a,24,25-pentol   | 18.275 | 438.3321 | 27-nor-5b-cholestane-3a,7a,12a,24,25-pentol   | C26 H46 O5       | C26 H46 O5       | C26 H46 O5       | 5.51   | 1  |
| Cpd 196: 18.675  | 18.675 | 478.0644 |   |                  |                  |                  |        |    |
| Cpd 197: 18.686  | 18.686 | 636.2949 |   |                  |                  |                  |        |    |
| Cpd 198: Epigallocatechin gallate  | 19.283 | 458.0814 | Epigallocatechin gallate  | C22 H18 O11      | C22 H18 O11      | C22 H18 O11      | 7.58   | 3  |
| Cpd 199: 19.283  | 19.283 | 478.0644 |   |                  |                  |                  |        |    |
| Cpd 200: S-(p-Azidophenacyl)glutathione  | 19.795 | 466.1204 | S-(p-Azidophenacyl)glutathione  | C18 H22 N6 O7 S  | C18 H22 N6 O7 S  | C18 H22 N6 O7 S  | 14.3   | 2  |

| Compound Label         | Name            | m/z      | RT    | Algorithm                 | Mass     |
|------------------------|-----------------|----------|-------|---------------------------|----------|
| Cpd 1: isoamyl nitrite | isoamyl nitrite | 118.0857 | 0.505 | Find by Molecular Feature | 117.0783 |